

Computing invariant measures with dimension reduction methods

Jens Kemper*

November 13, 2008

Abstract

We present an algorithm to compute invariant measures in high dimensions, e.g. in discretizations of scalar reaction diffusion equations. The algorithm combines subdivision techniques developed by Dellnitz, Junge and co-authors with Proper Orthogonal Decomposition as a model reduction method. Since the algorithm computes discrete measures with support in a low dimensional subspace of the state space we present methods for representing and comparing such measures. One such method aims at a discretization of the Prohorov metric. The paper also contains numerical results of the algorithms.

1 Introduction

In this paper we describe a feasible ansatz for the computation of invariant measures in high dimensional dynamical systems. More precisely, we consider the discrete dynamical system defined by

$$u_{i+1} = F(u_i), \quad i = 0, 1, 2, \dots$$

where F is a diffeomorphism of \mathbb{R}^N with large $N \gg 1$. Typically these large discrete dynamical systems arise from spatial discretizations of partial differential equations (see section 7 for details).

When we explore the longtime behavior of dynamical systems there are in principle two classical numerical approaches. One uses the simulation of many trajectories over large time intervals and in this way tries to get an overall picture of the dynamics. The disadvantage of this ansatz is that one cannot be sure to fetch all information of the long time behavior by this simulation technique. For example think of almost invariant sets in which trajectories are captured for long time scales.

The second approach is to make a global statistical analysis of the underlying system, for example the computation of invariant measures of the system. Denote by $\mathcal{M}_N = \mathcal{M}(\mathbb{R}^N)$ the set of probability measures on \mathbb{R}^N and recall that a measure $\mu \in \mathcal{M}_N$ is called F -invariant iff

$$\mu(A) = \mu(F^{-1}(A)) \quad \text{for all } A \in \mathcal{B}(\mathbb{R}^N).$$

The Frobenius-Perron Operator $P : \mathcal{M}_N \rightarrow \mathcal{M}_N$ is defined by

$$P(\mu)(A) = \mu(F^{-1}(A)) \quad \text{for all } A \in \mathcal{B},$$

such that fixed points of P are invariant measures.

For numerical computations one approximates the Frobenius-Perron operator by large matrices and computes eigenvectors to the eigenvalue 1 which lead to approximate invariant

*Supported by CRC 701 "Spectral Analysis and Topological Methods in Mathematics"

measures. In recent years a promising approach was developed by Dellnitz, Junge and co-workers. ([DFJ01], [DJ98], [DJ99]) This ansatz uses Ulam's method ([Ula60]) which basically means, that the state space is discretized into a box covering, from which one computes transition probabilities that represent the discretized version of the Frobenius-Perron operator. By rather efficient storing algorithms for the boxes and using an adaptive way of bisecting boxes this technique is a powerful tool to compute invariant measures in systems of low dimension. Details of this algorithm will be explained later.

However, when used in higher dimension this subdivision algorithm, called 'Adaptive Invariant Measure (AIM) algorithm', suffers from the 'curse of dimension'. Even when the support of the invariant measure is low-dimensional, the subdivision algorithm has to deal with an exponentially increasing number of boxes in the first recursion steps. If the state space is N -dimensional 2^N boxes are created to derive the first discretization in every coordinate. Since no relevant reduction can be expected before this step, the number of boxes quickly exceeds a computable amount even though the relevant dynamics is embedded in a low dimensional manifold.

There are several ways to approach this problem. We briefly discuss three of them.

- One can simplify the computation of invariant measures by using structure properties of the underlying system. Dellnitz and co-workers have presented an ansatz using symmetries of the dynamical system ([MHvMD06], [Jun01b]). They showed, that the symmetries of the system are linked to the symmetries of eigenmeasures of the Perron-Frobenius operator. This observation can in principle be used to derive these eigenmeasures with less computational costs.
- A new ansatz by Junge and Koltai [JK] uses so-called sparse hierarchical grids which are based on a tensor product construction. Using the Haar basis of $L^2([0, 1]^N)$ finite dimensional approximation spaces (given by a sparse basis) are derived which have the largest benefit to cost ratio. It can be shown that by this ansatz the computational effort is of significantly lower order than for the standard Ulam basis to achieve a comparable accuracy of the approximation.
- Another ansatz, that we follow here, is based on model reduction methods. We focus on the so-called Proper Orthogonal Decomposition (POD). This method is described for instance in [HLB96]. There are many promising results when using this method for the computation of single trajectories mainly in control theory (see [KV01], [KV02]). For linear systems they can also be combined with a balanced truncation ansatz ([Ant05], [ASG01], [RCM04]). In this paper we will use POD to approximate the global dynamics of a high-dimensional system.

The outline of this paper is as follows. In section 2 we briefly recall the subdivision algorithm, called Adaptive Invariant Measure algorithm, described in [DFJ01], [DJ98] and implemented in the Software Package GAIO. In section 3 we introduce the model reduction method of Proper Orthogonal Decomposition and explain how we combine this technique with the subdivision algorithm.

Since the approximate invariant measures that are computed by this algorithm live on a lower dimensional subspace of the original state space, given by the POD basis, it is nontrivial to represent and compare measures for different POD bases and the approximative invariant measure of the original subdivision algorithm respectively. Therefore we develop a proper representation of these discrete measures in section 4. Then in section 5 we discuss the Prohorov metric, that generates the weak-* topology. We will set up a numerical method for computing the distance of two measures in the Prohorov metric, which even works when the measures are supported on different POD spaces.

We develop in section 6 a more sophisticated version of our algorithm where the POD basis is adaptively changed during the subdivision process.

In section 7 we will present some numerical results concerning the approximation of invariant measures in a Chaffee-Infante problem and a more academic example where the

Lorenz system is embedded into a high dimensional system.

2 Adaptive invariant measure algorithm

We recall some basic steps of the set-oriented methods developed by Dellnitz, Junge et al. ([DFJ01], [DJ98]). The Adaptive Invariant Measure algorithm (AIM algorithm) adaptively refines box coverings of a positive invariant starting box. On these box collections discrete measures are computed as fixed points of discretized Perron-Frobenius operators. For later reference in section 3 we present a simple version of this algorithm.

The AIM algorithm

- **Initialization:** Let B_0 be a positive invariant box with center $c \in \mathbb{R}^N$ and radius $r \in \mathbb{R}^N$

$$B_0 := B(c, r) := \{x \in \mathbb{R}^N : |x_i - c_i| \leq r_i, i = 1, \dots, N\}.$$

The initial box collection is $\mathcal{B}_0 = \{B_0\}$ and the initial discrete measure $\mu_0 : \mathcal{B}(\mathbb{R}^N) \rightarrow [0, 1]$ is defined by

$$u_0(A) = \frac{\lambda_N(A \cap B_0)}{\lambda_N(B_0)}, \quad A \in \mathcal{B}(\mathbb{R}^N),$$

where λ_N is the N -dimensional Lebesgue measure.

- **Recursion step:** Assume that a partition \mathcal{B}_{k-1} of a subset of B_0 is given with a discrete measure $\mu_{k-1} : \mathcal{B}(\mathbb{R}^N) \rightarrow [0, 1]$.

1. Choose a subset $\mathcal{B}^{(1)}$ of \mathcal{B}_{k-1} where the actual measure is above average

$$\mathcal{B}^{(1)} = \{B \in \mathcal{B}_{k-1} : \mu_{k-1}(B) \geq 1/|\mathcal{B}_{k-1}|\}.$$

Subdivide boxes in $\mathcal{B}^{(1)}$ in coordinate $(k \bmod N)$ into a refined box collection $\mathcal{B}^{(2)}$ and continue with

$$\widehat{\mathcal{B}}_k := (\mathcal{B}_{k-1} \setminus \mathcal{B}^{(1)}) \cup \mathcal{B}^{(2)}, K := |\widehat{\mathcal{B}}_k|.$$

2. Calculate a normalized fixed point $u \in \mathbb{R}^K$, $\|u\|_1 = 1$ of the Frobenius-Perron matrix $P_k = (p_{ij})_{ij} \in \mathbb{R}^{K,K}$ defined by

$$p_{ij} = \frac{\lambda(B_j \cap F^{-1}(B_i))}{\lambda(B_j)}, \quad 1 \leq i, j \leq K. \quad (1)$$

where $\widehat{\mathcal{B}}_k = \{B_1, \dots, B_K\}$.

3. Set

$$\mathcal{B}_k = \{B_i \in \widehat{\mathcal{B}}_k : i = 1, \dots, K \text{ and } u_i > 0\} \subset \widehat{\mathcal{B}}_k$$

A new discrete measure $\mu_k : \mathcal{B}(\mathbb{R}^N) \rightarrow [0, 1]$ is defined by

$$\mu_k(A) = \sum_{i=1}^K u_i \frac{\lambda_N(A \cap B_i)}{\lambda_N(B_i)}, \quad A \in \mathcal{B}(\mathbb{R}^N).$$

It is easy to see, that the Frobenius-Perron matrix defined by (1) is column stochastic in

the sense

$$\sum_{i=1}^K p_{ij} = 1, \quad \text{for all } j = 1, \dots, K$$

since we assume B_0 to be positive invariant under F . Then the following theorem ensures the existence of a fixed point - or in other words the existence of an eigenvector to the eigenvalue $1 = \rho(P)$ with nonnegative entries.

Theorem 2.1 ([Min88]). *Let A be a real matrix with nonnegative entries. Then the following statements hold:*

- *The spectral radius $r := \max\{|\lambda| : \lambda \text{ is eigenvalue of } A\}$ is an eigenvalue of A .*
- *There is an eigenvector to the eigenvalue r with nonnegative entries.*
- *The estimate $\min_i \sum_j a_{ij} \leq r \leq \max_i \sum_j a_{ij}$ holds*

The discrete measure μ_k is absolutely continuous with density $u_k : \mathbb{R}^N \rightarrow [0, 1]$ defined by

$$u_k := \sum_{i=1}^K \frac{u_i}{\lambda_N(B_i)} \mathbb{1}_{B_i}$$

where $\mathbb{1}_A$ is the characteristic function of the set $A \subset \mathbb{R}^N$:

$$\mathbb{1}_A(x) = \begin{cases} 1, & x \in A \\ 0, & \text{otherwise} \end{cases}$$

Together with

$$\mu_k(\mathbb{R}^N) = \sum_{i=1}^K u_i = 1$$

this shows, that μ_k is a probability measure.

A convergence result based on the theory of small random perturbations can be found in [Jun01a]. Roughly speaking, the result states that the AIM algorithm, when applied to a system with sufficiently small noise, generates an approximate invariant measure that is close to the SRB measure of the deterministic system. For details on such small random perturbations see [Kif86].

3 Proper Orthogonal Decomposition

The concept of Proper Orthogonal Decomposition is used to produce reduced-order models mainly in problems arising in control theory. The idea is to determine a nested family of subspaces in the original state space that optimally span the data consisting of given snapshots. Usually these snapshots are derived from trajectories of the system.

3.1 Formulation of POD

The formal definition of the Proper Orthogonal Decomposition can be formulated in an arbitrary Hilbert space H , see [HLB96]

Definition 3.1. *Let $y_1, \dots, y_n \in H$ be a collection of snapshots. An l -dimensional orthonormal system $\{\psi_k\}_{k=1, \dots, l}$ is called proper orthogonal decomposition basis of rank l if it solves the minimization problem*

$$E(\{\psi\}_{k=1}^l) := \sum \|y_j - \sum_{k=1}^l (y_j, \psi_k)_H \psi_k\|_H^2 \text{ minimized over orthonormal bases.}$$

Theorem 3.2. Let $W := \text{span}\{y_1, \dots, y_p\} \subset H$. Let $\sigma_1 \geq \dots \geq \sigma_m > 0$, $m = \dim W$, be the singular values and let $w_1, \dots, w_m \in W$ be the corresponding singular vectors of the linear map $U \in L(\mathbb{R}^p, W)$ defined by

$$U(v) = \sum_{j=1}^p (v, e_j) y_j$$

where e_j are the Cartesian basis vectors of \mathbb{R}^p . Then $\{w_k\}_{k=1, \dots, l}$ is a POD basis of rank $l \leq m$ with error

$$E(\{w_k\}_{k=1, \dots, l}) = \sum_{k=l+1}^m \sigma_k^2.$$

(see [KV01], [HLB96])

In our context we take $H = \mathbb{R}^N$ and therefore, $U \in \mathbb{R}^{N,p}$ is just the matrix with the snapshots $y_1, \dots, y_p \in \mathbb{R}^N$ as columns.

3.2 The AIM algorithm in reduced space

The easiest way to combine POD as a reduction method with invariant measure algorithms is to compute a basis in the first step and apply the algorithm in the reduced system. We will propose this ansatz in the following algorithm

The PODAIM algorithm

- **Snapshots** For randomly chosen points $u_1^{(0)}, \dots, u_p^{(0)} \in B_0$ compute short trajectories to get test points

$$u_j = F^q(u_j^{(0)}), \quad j = 1 \dots, p.$$

- **POD computation** By a singular value decomposition of $U \in \mathbb{R}^{N,p}$ with columns u_1, \dots, u_p we get

$$(S \ 0) = W^T U V$$

with

$$S = \text{diag}(\sigma_1, \dots, \sigma_N) \in \mathbb{R}^{N,N}, \quad \sigma_1 \geq \dots \geq \sigma_N \geq 0$$

where $W \in \mathbb{R}^{N,N}, V \in \mathbb{R}^{p,p}$ are orthogonal. We choose $l \ll N$ e.g. by finding the smallest l with $\frac{\sigma_{l+1}}{\sigma_1} \leq \varepsilon$ and split $W = (W_1 \ W_2)$ with $W_1 \in \mathbb{R}^{N,l}$ and $W_2 \in \mathbb{R}^{N,N-l}$

- **AIM algorithm in POD space** A vector $u \in \mathbb{R}^N$ in the subspace defined by W_1 is represented by $\alpha \in \mathbb{R}^l$ via $u = W_1 \alpha$. We define a lower dimensional discrete dynamical system by

$$\alpha_{i+1} = W_1^T F(W_1 \alpha_i) \in \mathbb{R}^l$$

For this dynamical system we choose a proper positive invariant starting box and apply the AIM algorithm described in 2 to obtain a discrete measure $\mu_l : \mathcal{B}(\mathbb{R}^l) \rightarrow [0, 1]$ defined by

$$\mu_l(A) = \sum_{i=1}^K u_i \frac{\lambda_l(A \cap B_i)}{\lambda_l(B_i)}, \quad A \in \mathcal{B}(\mathbb{R}^l) \quad (2)$$

where $\{B_i\}_{i=1}^K$ is the box collection in the reduced space obtained by the AIM algorithm.

- **Embedding** A box $B = B(c, r) \subset \mathbb{R}^l$ can be embedded into the set $B^{W_1} \subset \mathbb{R}^N$ in the original space by the matrix W_1 :

$$B^{W_1} := \{z = W_1 x \in \mathbb{R}^N : x \in B\} = \{z = W_1 x \in \mathbb{R}^N : |x_i - c_i| \leq r_i, i = 1, \dots, l\}$$

These embedded boxes form the support of the extended measure $\mu_N : \mathcal{B}(\mathbb{R}^N) \rightarrow [0, 1]$ defined by

$$\mu_N(A) = \sum_{i=1}^K u_i \frac{\lambda_l(A \cap B_i^{W_1})}{\lambda_l(B_i^{W_1})}, \quad A \in \mathcal{B}(\mathbb{R}^N). \quad (3)$$

Remark 3.3. 1. In (3) we denote by λ_l the Lebesgue measure on the l -dimensional subspace $\text{span}\{w_1, \dots, w_l\}$ of \mathbb{R}^N . We have $\lambda_l(B_i^{W_1}) = \lambda_l(B_i)$ and

$$\lambda_l(A \cap B_i^{W_1}) = \lambda_l(\{x \in B_i : W_1 x \in A\}) = \lambda_l(B_i \cap W_1^{-1}(A))$$

where $W_1^{-1}(A) = \{x \in \mathbb{R}^l : W_1 x \in A\}$ denotes the preimage of A under W_1 . Therefore, μ_N can also be expressed as

$$\mu_N(A) = \sum_{i=1}^K u_i \frac{\lambda_l(B_i \cap W_1^{-1}(A))}{\lambda_l(B_i)}.$$

2. Observe that in contrast to the measure μ_l in the reduced system given by (2), the extended measure μ_N is not absolutely continuous. This is revealed by an alternative definition of μ_N that also shows the measure property of μ_N . Therefore let $\delta_0 : \mathcal{B}(\mathbb{R}) \rightarrow [0, 1]$ denote the onedimensional Dirac measure (cf. [Bau92], §25). Define

$$\tilde{\mu}_N = \mu_l \otimes \bigotimes_{j=l+1}^N \delta_0$$

where $\mu_1 \otimes \mu_2$ denotes the product measure of μ_1, μ_2 according to [Bau92], Def. 23.4. Then an alternative definition of μ_N is given by the transformation of $\tilde{\mu}_N$ via the orthogonal matrix $W \in \mathbb{R}^{N,N}$:

$$\mu_N(A) = \tilde{\mu}_N(W^T(A)), \quad A \in \mathcal{B}(\mathbb{R}^N).$$

Several extensions and problems of this first naive approach will be discussed in the following sections.

We are facing two problems when we examine the results of the PODAIM algorithm.

- Representing discrete measures in a high dimensional state space. We will present an ansatz in the following section which uses our assumption that a point in our state space corresponds to a spatial discretized solution $u : [0, 1] \rightarrow \mathbb{R}$ of a parabolic equation at a fixed time. We will introduce a suitable histogram over the unit interval.
- Comparison of discrete measures embedded in a high dimensional space with lower dimensional support. We will show in section 5, that usual discretizations of the weak metric do not work in our context but that the Prohorov metric is a suitable distance of measures that can be computed numerically.

4 Representing discrete measures in high dimensions

As described in the previous section the result of our algorithm is a discrete measure $\mu_N : \mathcal{B}(\mathbb{R}^N) \rightarrow [0, 1]$ with support on a box collection in an l -dimensional subspace of our state space \mathbb{R}^N given by (3).

Since we are focussing on Finite Element discretizations of scalar parabolic equations, in our context a state $u \in \mathbb{R}^N$ corresponds to a piecewise linear function $u : [0, 1] \rightarrow \mathbb{R}$ given by

$$u\left(\frac{i}{N+1}\right) = u_i, \quad i = 1, \dots, N, \quad u(0) = u(1) = 0.$$

This motivates the following representation.

4.1 Histogram

Recall the starting box in our phase space $B_0 = B(c, r)$ and set $r_M = \max_{0 \leq i \leq N} r_i$. We divide the set

$$Q = \left[\frac{1}{2(N+1)}, \frac{2N+1}{2(N+1)} \right] \times [-r_M, r_M] \subset \mathbb{R}^2$$

into a collection of boxes as follows

$$Q = \bigcup_{i=1}^N \bigcup_{j=1}^J Q_{ij}$$

where

$$Q_{ij} = \left[\frac{2i-1}{2(N+1)}, \frac{2i+1}{2(N+1)} \right] \times \left[(2(j-1) - J) \frac{r_M}{J}, (2j - J) \frac{r_M}{J} \right] =: R_i \times S_j.$$

Then we count those support boxes of our discrete measure whose i -th center component is in the corresponding interval to get a function $h : Q \subset \mathbb{R}^2 \rightarrow \mathbb{R}$ defined by

$$h(Q_{ij}) = \sum_{k=1}^K u_k \mathbb{1}_{Q_{ij}}\left(\frac{i}{N+1}, (W_1 c_k)_i\right) = \sum_{k=1}^K u_k \mathbb{1}_{S_j}\left((W_1 c_k)_i\right)$$

where $B_k = B_k(c_k, r_k) \subset \mathbb{R}^l$, $k = 1, \dots, K$ denote the support boxes with center c_k and radius r_k .

We can interpret h as a histogram operator since $h(Q_{ij})$ approximates

$$\mu_N(A_{ij}), \quad A_{ij} := \mathbb{R}^{i-1} \times S_j \times \mathbb{R}^{N-i}$$

Note that

$$\begin{aligned} \mu_N(A_{ij}) &= \sum_{k=1}^K u_k \frac{\lambda_l(A_{ij} \cap B_k^{W_1})}{\lambda_l(B_k^{W_1})} \\ &= \sum_{k=1}^K u_k \frac{\lambda_l(\{x \in B_k^{W_1} : x_i \in S_j\})}{\lambda_l(B_k^{W_1})} \\ &\approx \sum_{k=1}^K u_k \begin{cases} 1, & \text{if } ((c(B_k^{W_1}))_i) = (W_1 c_k)_i \in S_j \\ 0, & \text{otherwise} \end{cases} \\ &= h(Q_{ij}) \end{aligned}$$

where $c(B^W)$ denotes the center of an embedded box $B^W \subset \mathbb{R}^N$. Here the approximation process is reasonable because in general $\text{diam}(B^W) \ll 2 \frac{r_M}{J} = \text{diam}(S_j)$ holds for the

support boxes $B^W \subset \mathbb{R}^N$ and, therefore, most boxes either lie in A_{ij} or in its complement as indicated by the center.

With this discrete representation operator we visualize our results by color coding Q_{ij} according to the value $h(Q_{ij})$. It is easy to see, that the corresponding matrix $H = (h(Q_{ij}))_{ij}$ is stochastic if the support boxes are located in B_0

$$\begin{aligned} \sum_{j=1}^J h(Q_{ij}) &= \sum_{k=1}^K u_k \sum_{j=1}^J \mathbb{1}_{Q_{ij}}(i, (W_1 c)_i) \\ &= \sum_{B=B(c,r) \in \mathcal{B}} u_k(B) = 1 \end{aligned}$$

For examples we refer to section 7.

5 Comparing discrete measures: Prohorov metric

In this section we develop an algorithm for computing the distance of discrete measures obtained by our algorithm.

Recall that the support of μ_N in the PODAIM algorithm is given by a low dimensional box collection $\mathcal{B} = \{B_1, \dots, B_K\}$ embedded in an l -dimensional subspace $\text{span}W$ as boxes $B_k^W \subset \mathbb{R}^N$, $k = 1, \dots, K$. With these boxes $\mu_N : \mathcal{B}(\mathbb{R}^N) \rightarrow [0, 1]$ is defined by (3).

Our aim is to compare measures for different choices of $l \leq N$ and different POD bases $W \in \mathbb{R}^{N,l}$ including the measure of the AIM algorithm where $l = N$ and $W = I_N$ is the identity matrix.

5.1 The weak-* topology

Recall that the space $\mathcal{M}(Q)$ of probability measures on a compact set Q defines a compact metric space via the weak-* metric $d_* : \mathcal{M}(Q) \times \mathcal{M}(Q) \rightarrow \mathbb{R}_+$ defined by

$$d_*(\mu, \nu) = \sum_{i=0}^{\infty} 2^{-i} \left| \int g_i d\mu - \int g_i d\nu \right|, \quad (4)$$

where $(g_i)_i$ is a dense sequence in $C(Q)$ (see [Dud02]).

If we apply this metric in our context to approximate $d_*(\mu_N, \nu_N)$, where the corresponding discrete measures μ and ν have support on box collections $\{A_j\}_j, \{B_k\}_k$ in the POD spaces defined by $W_1 \in \mathbb{R}^{N,l_1}$ and W_2^{N,l_2} , we have to choose a proper (finite) sequence of test functions $(g_i)_i$. Due to the shape of our discrete measures a natural choice is

$$\{\mathbb{1}_{A_1^{W_1}}, \dots, \mathbb{1}_{A_J^{W_1}}, \mathbb{1}_{B_1^{W_2}}, \dots, \mathbb{1}_{B_K^{W_2}}\}$$

However, one easily shows that the approximate weak-* distance is 1 as soon as the supports of the discrete measures are disjoint. Therefore we avoid using the definition (4) directly.

5.2 The concept of blowing up boxes

A more promising ansatz is given by the Prohorov metric which plays a role in theoretical aspects of probability theory. ([Dud02], [Bil68]). This metric is oriented geometrically.

Definition 5.1. *Let*

$$\mathcal{M}(S) := \{\mu : \mathcal{B} \rightarrow [0, 1] : \mu \text{ is a probability measure}\},$$

where S is a metric space with Borel σ -algebra \mathcal{B} . Define the Prohorov metric p by

$$p(\mu, \nu) = \inf\{\varepsilon > 0 : \mu(A) \leq \nu(A^\varepsilon) + \varepsilon \text{ and } \nu(A) \leq \mu(A^\varepsilon) + \varepsilon \text{ for all } A \in \mathcal{B}\} \quad (5)$$

where $\mu, \nu \in \mathcal{M}(S)$ and A^ε is the ε -neighborhood of A :

$$A^\varepsilon := \{x \in S : d(x, A) < \varepsilon\}.$$

Note the following well known result.

Theorem 5.2 ([Dud02]). *The mapping $p : \mathcal{M}(S) \times \mathcal{M}(S) \rightarrow \mathbb{R}_+$ defines a metric on the space of probability measures $\mathcal{M}(S)$. Moreover, p is equivalent to the weak- $*$ metric.*

We show that the Prohorov metric is well suited for numerical discretizations.

5.3 Implementation

Again we take the boxes of the supports as test sets for the discretized version of the Prohorov metric. Let $\mu_N, \nu_N : \mathcal{B}(\mathbb{R}^N) \rightarrow [0, 1]$ be two discrete measures on box collections $\mathcal{A} = \{A_j\}_{j=1, \dots, J} \subset \mathbb{R}^{l_1}$, $\mathcal{B} = \{B_k\}_{k=1, \dots, K} \subset \mathbb{R}^{l_2}$ embedded by $W_1 \in \mathbb{R}^{N, l_1}, W_2 \in \mathbb{R}^{N, l_2}$ into \mathbb{R}^N . (cf. (3))

$$\mu_N(A) = \sum_{j=1}^J u_j \frac{\lambda_{l_1}(A \cap A_j^{W_1})}{\lambda_{l_1}(A_j^{W_1})}, \quad \nu_N(A) = \sum_{k=1}^K v_k \frac{\lambda_{l_2}(A \cap B_k^{W_2})}{\lambda_{l_2}(B_k^{W_2})}, \quad A \in \mathcal{B}(\mathbb{R}^N).$$

Remember the definition $B^W = \{Wx \in \mathbb{R}^N : x \in B\}$. We discretize the analytic Prohorov distance $p(\mu_N, \nu_N)$ in two steps to get a computable version $p^{[2]}(\mu_N, \nu_N)$. In the first step, we replace $A \in \mathcal{B}$ by our boxes of the supports in definition (5) and get

$$p^{[1]}(\mu_N, \nu_N) = \max\{p_1^{[1]}(\mu_N, \nu_N), p_2^{[1]}(\mu_N, \nu_N)\}$$

with

$$p_1^{[1]}(\mu_N, \nu_N) = \inf\{\varepsilon > 0 : \mu_N(A_j^{W_1}) \leq \nu_N((A_j^{W_1})^\varepsilon) + \varepsilon\}.$$

The distance $p_2^{[1]}$ is defined analogous via the box collection $\{B_k^{W_2}\}_{k=1}^K$. We will focus on $p_1^{[1]}$ in the following, all implications will be the same for $p_2^{[1]}$.

By definition it holds

$$\mu_N(A_j^{W_1}) = \sum_{i=1}^J u_i \frac{\lambda_{l_1}(A_j^{W_1} \cap A_i^{W_1})}{\lambda_{l_1}(A_i^{W_1})} = u_j, \quad j = 1, \dots, J$$

and similarly $\nu_N(B_k^{W_2}) = v_k$, $k = 1, \dots, K$. This allows us to write $p_1^{[1]}$ as

$$p_1^{[1]}(\mu_N, \nu_N) = \inf\{\varepsilon > 0 : \max_{j=1, \dots, J} (u_j - \nu_N((A_j^{W_1})^\varepsilon) - \varepsilon) \leq 0\}.$$

In the next step we explain how to approximate

$$\nu_N((A_j^{W_1})^\varepsilon) = \sum_{k=1}^K v_k \frac{\lambda_{l_2}(B_k^{W_2} \cap (A_j^{W_1})^\varepsilon)}{\lambda_{l_2}(B_k^{W_2})}.$$

By a Monte-Carlo ansatz with P test points $b_1^k, \dots, b_P^k \in B_k$ we get

$$\frac{\lambda_{l_2}(B_k^{W_2} \cap (A_j^{W_1})^\varepsilon)}{\lambda_{l_2}(B_k^{W_2})} \approx \frac{1}{P} \#\{b_p^k : W_2 b_p^k \in (A_j^{W_1})^\varepsilon\} = \frac{1}{P} \#\{b_p^k : d(W_2 b_p^k, A_j^{W_1}) < \varepsilon\}$$

Now we approximate

$$\nu_N((A_j^{W_1})^\varepsilon) \approx w_j(\varepsilon) := \sum_{k=1}^K \frac{u_k}{p} \#\{b_i^k : d(W_2 b_i^k, A_j^{W_1}) < \varepsilon\}.$$

We will see below, that $d(W_2 b_p^k, A_j^{W_1})$ can be computed analytically. Then we approximate the Prohorov distance by

$$p_1^{[1]}(\mu_N, \nu_N) \approx p_1^{[2]}(\mu_N, \nu_N) := \begin{cases} \min\{\varepsilon > 0 : f_1(\varepsilon) = 0\}, & f_1(0) > 0 \\ 0, & \text{otherwise} \end{cases}$$

where $f_1; \mathbb{R}_+ \rightarrow \mathbb{R}$ is defined by

$$f_1(\varepsilon) = \max_{j=1, \dots, J} (\alpha_j - w_j(\varepsilon) - \varepsilon).$$

Since w_j is isotone for every $j = 1, \dots, J$, f_1 is antitone and we can compute the root of f e.g. by Newton's method to get $p_1^{[2]}(\mu_N, \nu_N)$.

The second value $p_2^{[2]}(\mu_N, \nu_N)$ can be computed in an analogous way by approximating $p_2^{[1]}(\mu_N, \nu_N)$.

Computation of the distances

Now we face the problem to compute

$$d(W_2 t, A^{W_1})$$

where $W_i \in \mathbb{R}^{N, l_i}$, $i = 1, 2$ are orthogonal matrices, $t \in \mathbb{R}^{l_2}$ and a box $A = B(c, r)$ with center and radius $c, r \in \mathbb{R}^{l_1}$ is projected to $A^{W_1} \subset \mathbb{R}^N$ via W_1 .

We set $t_1 = W_1^T(W_2 t) \in \mathbb{R}^{l_1}$. Because $W_2 t - W_1 t_1$ is orthogonal to the hyperplane containing $W_1 t_1$ and A^{W_1} we get for the Euclidean distance

$$d(W_2 t, A^{W_1})^2 = d(W_1 t_1, A^{W_1})^2 + \|W_2 t - W_1 t_1\|_2^2.$$

Now on the one hand we have

$$d(W_1 t_1, A^{W_1})^2 = d(t_1, A)^2 = \|d\|_2^2$$

where $d \in \mathbb{R}^{l_1}$ is given by

$$d_i = \max(0, |(t_1)_i - c_i| - r_i), \quad i = 1, \dots, l_1.$$

On the other hand we use orthogonality to get

$$\|W_2 t - W_1 t_1\|_2^2 = \|W_2 t\|_2^2 - \|W_1 t_1\|_2^2 = \|t\|_2^2 - \|t_1\|_2^2.$$

Altogether we obtain

$$d(W_2 t, A^{W_1})^2 = \|d\|_2^2 + \|t\|_2^2 - \|t_1\|_2^2.$$

Observe that only the lengths of low dimensional vectors $t \in \mathbb{R}^{l_2}$, $d, t_1 \in \mathbb{R}^{l_1}$ are used for the computation.

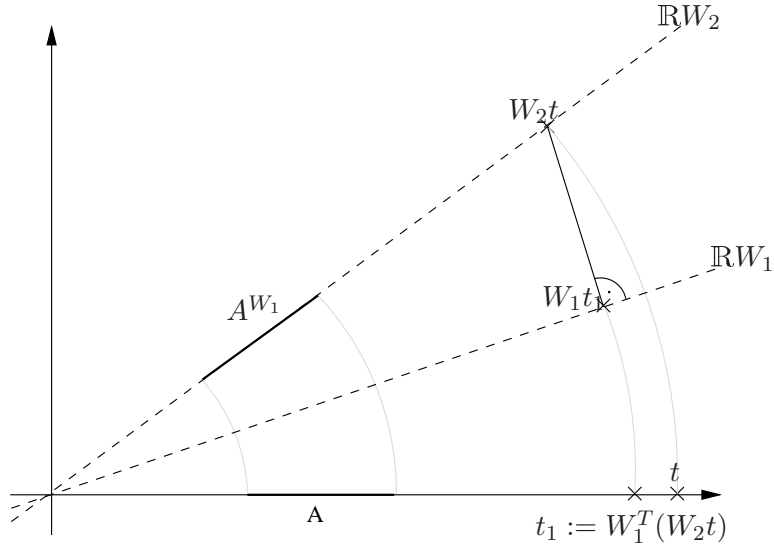


Figure 1: Illustration of the Euclidean distance computation needed for the approximation of the Prohorov distance. Here the spatial dimensions are given by $N = 1$, $l_1 = l_2 = 1$.

6 Adaptive POD algorithm

Looking closer at the original subdivision algorithm it is an obvious idea to compute the POD modes adaptively during the recursion steps of the AIM algorithm. Since the algorithm computes short time trajectories to build the transfer matrix, this data can be used to derive an adapted POD basis during the algorithm.

The algorithm PODADAPT works as follows. Instead of computing discrete measures in a fixed state space, also the POD subspace will be changed dynamically. Therefore we manage not only a box collection and a corresponding discrete measure but also the POD basis throughout the algorithm. We start with the original state space or in other words the canonical basis of \mathbb{R}^N as the first POD basis. After some recursion steps the computed trajectories are used to compute a new POD basis. Now the system is transformed into the new state space and a new box collection of comparable complexity is built in the new state space. Then the algorithm continues to work in the new state space.

In detail we suggest the following algorithm

The PODADAPT algorithm

- **Initialization:** Start with $W = I_N$, $l = N$. $\mathcal{B}_0 = \{Q\}$, $Q \subset \mathbb{R}^N$ positive invariant, $u_0 : \mathcal{B}_0 \rightarrow [0, 1]$ defined by $u_0(Q) = 1$.
- **Recursion step k :** Let \mathcal{B}_{k-1} a collection of boxes in the POD space given by $W \in \mathbb{R}^{N,l}$.
 1. **New box collection:** As in the original AIM algorithm calculate a new box collection \mathcal{B}_k of $J = |\mathcal{B}_k|$ boxes.

2. **Test points:** As in the AIM algorithm choose P random points in each box $B \in \mathcal{B}_k$

$$u_1^{(j)}, \dots, u_P^{(j)} \in B_k \subset \mathbb{R}^l, \quad j = 1, \dots, J.$$

and evaluate the modified right hand side for these vectors

$$v_p^{(j)} := F(Wu_p^{(j)}) \in \mathbb{R}^N.$$

3. **AIM algorithm:** Compute an approximation u_k of an invariant measure as in the POD algorithm from the fixed point of the Perron-Frobenius matrix $P = (p_{ij})_{ij}$ with

$$p_{ij} = \frac{1}{P} |\{W^T v_p^{(j)} \in B_i : p = 1, \dots, P\}|, \quad i, j = 1, \dots, J$$

4. **POD transformation:** After a fixed number of recursion steps compute a new POD basis in the following way:

- **POD snapshots** In each box choose image points the number of which is determined by the discrete measure u_k :

$$V := \{v_p^{(j)} : j = 1, \dots, J, p = 1, \dots, \lceil u_k(B_j) P \rceil\}$$

where $\lceil x \rceil$ is the smallest natural number above x .

- **POD basis:** Calculate a new POD basis $\widetilde{W} \in \mathbb{R}^{N, \tilde{l}}$ by a singular value decomposition of V . Choose $\tilde{l} < N$ in a reasonable way, e.g. such that the $\tilde{l} + 1$ largest singular value is smaller than a given tolerance.
- **Transformation:** After a given number of recursion steps (e.g. one in each space dimension) we transfer the system to a new \tilde{l} dimensional POD space given by \widetilde{W} using the following steps
 - (a) Determine the box $B = B(c, r) \in \mathcal{B}_k$ with the smallest diameter of the current collection and set $r_m := \min\{r_i : i = 1, \dots, l\}$.
 - (b) Create a box collection $\widehat{\mathcal{B}} = \{\widehat{B}_1, \dots, \widehat{B}_M\}$ as a covering of $\widetilde{W}^T Q$ where all boxes $\widehat{B}_i = \widehat{B}_i(c, r)$ have the same radius $r = (r_m, \dots, r_m)^T$.
 - (c) Eliminate all boxes not containing embedded test points:

$$\widetilde{\mathcal{B}} = \{B \in \widehat{\mathcal{B}} : B \cap \{\widetilde{W}v_p^{(j)} : j = 1, \dots, J, p = 1, \dots, P\} \neq \emptyset\}.$$

Continue with the new POD basis $W = \widetilde{W}$ of dimension $l = \tilde{l}$ and the box collection $\mathcal{B} = \widetilde{\mathcal{B}}$.

We will analyze this algorithm and compare with the results from the PODAIM algorithm in the following section.

7 Numerical results

We analyze our algorithms for two discrete dynamical systems. The first one is given by a generalization of the well-known Lorenz system. We will embed this system into a high dimensional space to see how the POD approximation process works.

In the second example we apply our algorithms to space-time discretizations of a parabolic equation. We choose the scalar Chafee-Infante problem which has a cubic nonlinearity. The discretization uses the Finite Element Method (FEM).

7.1 Embedded Lorenz system

We derive a discrete dynamical system from the following system of ODEs

$$u' = \begin{pmatrix} u_1' \\ u_2' \\ u_3' \\ u_4' \\ \vdots \\ v_N \end{pmatrix} = \begin{pmatrix} \sigma(u_2 - u_1) \\ \rho u_1 - u_2 - u_1 u_3 \\ u_1 u_2 - \beta u_3 \\ -\alpha u_4 \\ \dots \\ -\alpha u_N \end{pmatrix} =: F_L(u) \quad (6)$$

The first three equations of the system are just given by the Lorenz system ([Lor63]). We will use the 'standard' parameters $\sigma = 10$, $\rho = 28$, $\beta = 8/3$ in the following.

We take $\alpha > 0$ so that the remaining equations define exponentially decreasing components. A discrete dynamical system is derived from (6) by Euler discretization.

$$u_{i+1} = F_h(u_i), \quad F_h(v) = v + hF_L(v)$$

Now we embed the system into a quadratic manifold. Therefore we define $t_\varepsilon : \mathbb{R} \rightarrow \mathbb{R}$ by

$$t_\varepsilon(x) = (1 - \varepsilon)x + \varepsilon x^2.$$

Some analysis shows, that t_ε is a one-to-one mapping of $D_\varepsilon := (-\frac{1-\varepsilon}{2\varepsilon}, \infty)$ onto $R_\varepsilon := (-\frac{(1-\varepsilon)^2}{4\varepsilon^2}, \infty)$. The inverse function $t_\varepsilon^{-1} : R_\varepsilon \rightarrow D_\varepsilon$ is given by

$$t_\varepsilon^{-1}(y) = \sqrt{\frac{y}{\varepsilon} + \frac{(1-\varepsilon)^2}{4\varepsilon^2}} - \frac{1-\varepsilon}{2\varepsilon}.$$

With these scalar functions we can formulate a quadratic perturbation in higher systems via $T_\varepsilon : D_\varepsilon^N \rightarrow R_\varepsilon^N$ defined by

$$T_\varepsilon ps(v)_i = t_\varepsilon(v_i), \quad i = 1, \dots, N$$

with T_ε^{-1} defined in an analogue way via t_ε^{-1} . To randomize the orientation of the perturbation we transform the state space with some randomly chosen orthogonal matrix $Q \in \mathbb{R}^{N,N}$.

Altogether we get a discrete dynamical system

$$v_{i+1} = G_{h,\varepsilon}(v_i) := T_\varepsilon(QF_h(Q^T T_\varepsilon^{-1}(v_i))), \quad i = 1, \dots, N. \quad (7)$$

In Figure 2 we present the result of the PODAIM algorithm for the system (7) in dimension $N = 10$. The following parameter values have been used.

$$\begin{aligned} \sigma &= 10, \rho = 28, \beta = 8/3 \\ Q &\in \mathbb{R}^{N,N} \text{ with } Q^T Q = I_{10} \text{ and } Q \text{ has random entries} \\ \epsilon &= 0.001, \alpha = 0.9, h = 0.01 \end{aligned}$$

The largest singular values computed in step 2 were

$$\sigma_1 = 742.0957, \sigma_2 = 333.8305, \sigma_3 = 75.0522, \sigma_4 = 2.3911$$

Due to the gap in magnitude between σ_3 and σ_4 the POD dimension $l = 3$ was chosen.

It is reasonable that the resulting POD space, given by $W \in \mathbb{R}^{10,3}$, is located near the subspace spanned by the first three columns $Q_3 \in \mathbb{R}^{10,3}$ of the linear transformation Q , since only a small quadratic perturbation was added to the state space. To measure the distance we compute the principal angles as defined in [GvL96] (Algorithm 12.4-3 and corresponding definition):

For general subspaces defined by $A \in \mathbb{R}^{m,q}$, $B \in \mathbb{R}^{m,p}$, $q \geq p$, the cosine of the principle angles θ_k , $k = 1, \dots, q$ are given by the singular values of $C = Q_1^T Q_2$ where $A = Q_1 R_1$ and $B = Q_2 R_2$ are the QR decompositions of A and B respectively with $Q_1 \in \mathbb{R}^{q,q}$, $Q_2 \in \mathbb{R}^{p,p}$ orthonormal.

Since W and Q_3 are orthonormal in our case the principal angles are given by $\cos^{-1}(\sigma_k)$, $k = 1, 2, 3$, where σ_k are the singular values of $W^T Q_3$. As expected the principal angles are small:

$$\theta = (0.0009, 0.0034, 0.0111)^T.$$

The Figure 2 shows the resulting box collection in the POD space after $k = 27$ recursion steps.

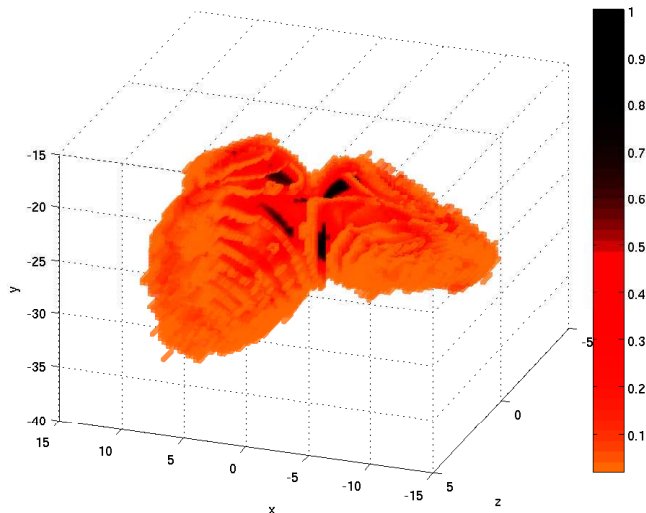


Figure 2: Resulting box collection of PODAIM algorithm for the embedded Lorenz system in $N = 10$ dimensions.

7.2 Scalar Chafee-Infante problem

We apply our algorithm to a dynamical system arising from the discretization of the scalar Chafee-Infante problem with a cubic nonlinearity

$$u_t = u_{xx} - \lambda(u^3 - u), \quad 0 < x < 1, \quad t > 0, \quad (8)$$

$$u(0, t) = u(1, t) = 0, \quad t > 0 \quad (9)$$

Before we can apply our algorithms we have to fully discretize the parabolic system.

Finite Elements

For the spatial discretization we choose a Standard Finite-Elements ansatz (cf. [LT03]) with linear basis functions. Therefore let $x_i = ih$, $i = 1, \dots, N$ be the equally distributed grid

points in the unit interval with step size $h = \frac{1}{N+1}$. We choose piecewise linear basis functions $\Lambda_j : [0, 1] \rightarrow \mathbb{R}$ given by

$$\Lambda_j(x_i) = \delta_{ij}, \quad (i, j \in \{1, \dots, N\})$$

By the weak formulation in $V_h := \text{span}\{\Lambda_1, \dots, \Lambda_N\}$ one gets the condition for the finite element solution $u_h \in V_h$ by

$$\left(\frac{d}{dt}u_h(t), \Lambda_j\right)_2 + a(u_h(t), \Lambda_j) = \lambda(u_h(t))^3 - u_h(t), \Lambda_j)_2, \quad (1 \leq j \leq N)$$

with the elliptic form

$$a(u, v) = \int_0^1 u' v' dx, \quad (u, v \in V_h).$$

Using the representation $u_h(t) = \sum_{i=1}^N \alpha_i(t) \Lambda_i \in V_h$ one gets a system of ODEs

$$B_h \alpha'(t) + A_h \alpha = \lambda G_h(\alpha(t)). \quad (10)$$

where $B_h = ((\Lambda_j, \Lambda_i)_2)_{ij} \in \mathbb{R}^{N,N}$ is the mass matrix and $A_h = (a(\Lambda_j, \Lambda_i))_{ij} \in \mathbb{R}^{N,N}$ the stiffness matrix. Further on, the nonlinear function $G : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is defined by

$$G_h(\alpha)_j = \int_0^1 \Lambda_j(x) \left\{ \left(\sum_{i=1}^N \alpha_i \Lambda_i(x) \right)^3 - \sum_{i=1}^N \alpha_i \Lambda_i(x) \right\} dx \quad (11)$$

We derive an explicit formula from (10) by inserting the formulas for the basis functions Λ_j . Then we get

$$B_h = \frac{h}{6} B, \quad A_h = \frac{1}{h} A, \quad G_h(\alpha) = h G(\alpha)$$

with

$$B = \begin{pmatrix} 4 & 1 & & & \\ 1 & \ddots & \ddots & & \\ & \ddots & \ddots & 1 & \\ & & & 1 & 4 \end{pmatrix}, \quad A = \begin{pmatrix} 2 & -1 & & & \\ -1 & \ddots & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & & -1 & 2 \end{pmatrix},$$

$$G(\alpha)_j = \frac{\alpha_{j-1}}{6} + \frac{2\alpha_j}{3} + \frac{\alpha_{j+1}}{6} - \frac{\alpha_{j-1}^3}{20} - \frac{2\alpha_j^3}{5} - \frac{\alpha_{j+1}^3}{20} - \frac{\alpha_{j-1}^2 \alpha_j}{10} - \frac{3\alpha_{j-1} \alpha_j^2}{20} - \frac{3\alpha_j^2 \alpha_{j+1}}{20} - \frac{\alpha_j \alpha_{j+1}^2}{10}$$

This leads to the following explicit ODE (note $\frac{1}{h} = N + 1$)

$$\alpha'(t) = 6B^{-1}(-(N+1)^2 A \alpha(t) - \lambda G(\alpha(t))). \quad (12)$$

For the time discretization we take the explicit Euler method and derive from (12) a discrete dynamical system that we will analyze with our algorithms described above:

$$\alpha_{i+1} = F(\alpha_i), \quad i = 1, 2, \dots, \quad (13)$$

where $F : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is defined by

$$F(\alpha) = \alpha + \frac{1}{\Delta t} (6B^{-1}(-(N+1)^2 A \alpha - \lambda G(\alpha))).$$

Note that we have to satisfy the stability restriction

$$\frac{\Delta t}{h^2} \leq \frac{1}{2} \iff \Delta t \leq \frac{1}{2(N+1)^2}.$$

The dynamical behavior of the continuous problem is well-analyzed, see for instance [Hen81], [Rob01]. Depending on the parameter $\lambda > 0$ the fixed-points of (8) are described by the following theorem.

Theorem 7.1. *Let $n \in \mathbb{N}$ be given with $n^2\pi^2 < \lambda < (n+1)^2\pi^2$. Then the following holds*

- *The continuous Chafee-Infante problem (8) possesses $2n+1$ fixed points $\phi_0, \phi_1^\pm, \dots, \phi_n^\pm$*
- *ϕ_0 is just the trivial solution and ϕ_k^+ and ϕ_k^- are symmetric with $\frac{d}{dx}\phi_k^+ > 0$ and $\frac{d}{dx}\phi_k^- < 0$ respectively. Moreover $\phi_{k\pm}$ has $k-1$ zeros in $(0,1)$ at*

$$\frac{1}{k}, \frac{2}{k}, \dots, \frac{k-1}{k}$$

- *For $n=0$ the only fixed point ϕ_0 is stable. For $n \geq 1$ we have 2 stable fixed points ϕ_1^\pm and $2n-1$ unstable fixed points ϕ_0 and $\phi_k^\pm, 2 \leq k \leq n$.*

One can also construct an absorbing set for the Chafee-Infante problem. By that the existence of a global attractor \mathcal{A} in the Sobolev space $H_0^1([0,1])$ is guaranteed. Further on, the existence of a Lyapunov function on the global attractor gives a detailed description of the global attractor.

Theorem 7.2 ([Rob01]). *The global attractor \mathcal{A} of the Chafee-Infante problem is given by the union of the unstable manifolds of its fixed points:*

$$\mathcal{A} = \bigcup \{W^u(\phi) : \phi \in \{\phi_0, \phi_1^\pm, \dots, \phi_n^\pm\}\}.$$

where ϕ_i^\pm are the fixed points defined in theorem 7.1 and $W^u(v)$ denotes the unstable manifold of v .

The convergence theory of Finite Element discretizations of semilinear parabolic equations ([LSS94], [Lar99]) leads to the same shape of the attractor for the spatially discretization because the existence of a Lyapunov function and an absorbing set transfers with slightly perturbed bifurcation points.

It is known that the support of all invariant measures is a subset of the global attractor, see [CKR08], where this result is shown for modified Navier-Stokes equations. More precisely we will see below, that the support sets of the discrete measures we obtain from the set-oriented algorithms consist of small neighborhoods of the non-trivial fixed points. This is due to the fact that the unstable manifolds between the fixed points are not part of the support of SRB measures approximated by the AIM algorithm.

Multiple eigenvalue 1 of the Perron-Frobenius matrix

Recall that the Perron-Frobenius theorem 2.1 for nonnegative matrices guarantees the existence of the eigenvalue 1 of the Perron-Frobenius matrix and of a corresponding nonnegative eigenvector.

In the context of the transfer operator each Dirac measure of a fixed point corresponds to an eigenvector to the eigenvalue 1 of the Perron-Frobenius matrix P . That means that we have to face the problem of a geometrically multiple eigenvalue 1 of P . In order to obtain as much as possible of the dynamics of our system we are interested in a equally weighted linear combination of the eigenvectors corresponding to the Dirac measures as a representation of the discrete measure.

Recall that the Perron-Frobenius theorem 2.1 for nonnegative matrices guarantees the existence of the eigenvalue 1 of the Perron-Frobenius matrix and of a corresponding nonnegative eigenvector. Typical eigenproblem solvers (e.g. `eigs` in `MATLAB`) will give us an orthonormal basis $\{v_1, \dots, v_k\}$ of the eigenspace to the eigenvalue 1. But in general these vectors may

have negative entries although there exists a basis of nonnegative vectors corresponding to the Dirac measures.

Hence we setup an algorithm to transfer the orthonormal basis $\{v_1, \dots, v_k\}$ to another orthonormal basis $\{p_1, \dots, p_k\}$ with nonnegative vectors p_i . If we arrange the vectors in matrices $V \in \mathbb{R}^{N,k}$ and $P \in \mathbb{R}^{N,k}$ with columns v_i and p_i respectively we write

$$P = VO$$

where $O \in \mathbb{R}^{K,K}$ is an orthonormal matrix. For simplification we write O as a composition of rotation matrices

$$O = O_1(\alpha_1)O_2(\alpha_2) \cdots O_{k-1}(\alpha_{k-1})$$

with

$$\begin{aligned} O_l(\alpha) &= (o_{ij})_{ij}, \\ o_{i,j \in \{l, l+1\}} &= \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) \\ \sin(\alpha) & \cos(\alpha) \end{pmatrix}, \\ o_{ij} &= \delta_{ij}, \quad i \notin \{l, l+1\} \text{ or } j \notin \{l, l+1\} \end{aligned}$$

In this way we rotate the basis vectors one by one into the cone of nonnegative vectors. Therefore we minimize the following function to get the angles $\alpha_l, l = 1, \dots, k-1$:

$$\begin{aligned} f_l(\alpha) &= \min\left(\sum\{p_{il} : p_{il} > 0, i = 1, \dots, k\}, -\sum\{p_{il} : p_{il} < 0, i = 1, \dots, k\}\right) \\ &\quad + \min\left(\sum\{p_{i, l+1} : p_{i, l+1} > 0, i = 1, \dots, k\}, -\sum\{p_{i, l+1} : p_{i, l+1} < 0, i = 1, \dots, k\}\right) \end{aligned}$$

where $P = (p_{ij}) = VO_1(\alpha_1) \cdots O_{l-1}(\alpha_{l-1})O_l(\alpha)$.

Then we expect that each column p_i of

$$P = VO_1(\alpha_1)O_2(\alpha_2) \cdots O_{k-1}(\alpha_{k-1})$$

is nonnegative and therefore a good approximation to a Dirac measure in a fixed point of the system. By summing up and normalizing the columns we get a suitable new fixed point u of P with $\|u\|_1 = 1$

$$u := \frac{v}{\|v\|_1}, \quad v = \sum_{i=1}^k p_i.$$

Results

As a first test example we compare the results of the AIM and the PODAIM algorithm on system (13) for the following parameters.

$$\begin{aligned} N &= 6 \\ \lambda &= 80 \\ \Delta t &= 0.001 \end{aligned}$$

From the bifurcation theory we expect 5 fixed points of the system that should be detected by the invariant measure algorithms. Due to symmetry these fixed points are located in a twodimensional subspace of \mathbb{R}^N . Indeed the PODAIM algorithm evolves a POD dimension of $l = 2$. In Figure 3 we see a histogram representating the discrete measure computed by the AIM algorithm after 66 subdivision steps, i.e. 11 bisections in each space dimension. The four nontrivial fixed points are well detected.

In Figure 4 we see the promising result that also in the POD space the fixed points are detected although their shape is slightly perturbed from the shape in the AIM algorithm. In

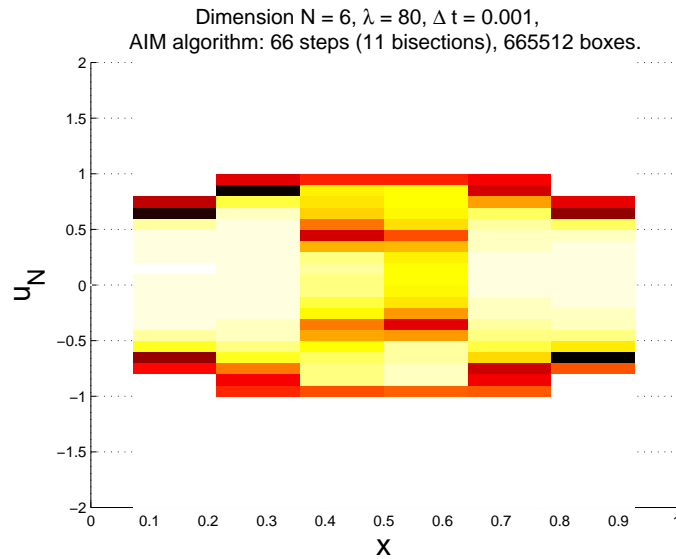


Figure 3: Resulting box collection of AIM algorithm for the Chafee-Infante problem in $N = 6$ dimensions with parameter $\lambda = 80$ after $k = 66$ subdivision steps.

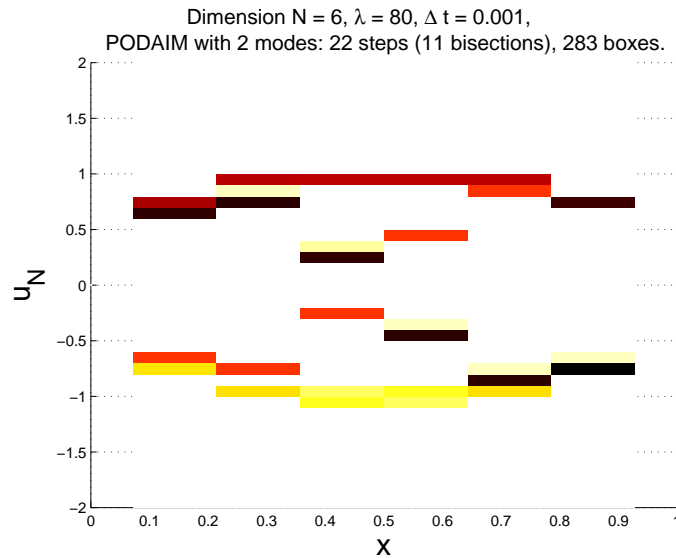


Figure 4: Resulting box collection of PODAIM algorithm for the Chafee-Infante problem in $N = 6$ dimensions with parameter $\lambda = 80$. The POD dimension is $l = 2$ and $k = 22$ subdivision steps are computed.

this figure the discrete measure is illustrated after $k = 22$ subdivision steps corresponding also to 11 bisections in each space dimension. The most remarkable result of this example is the number of boxes building the support of the two discrete measures. In the AIM algorithm - despite of the simple form of the approximated invariant measure - more than 600.000 boxes are building the support of the discrete measure while in the PODAIM algorithm only 283 boxes are needed to produce a similar result.

We can also quantify the difference of the discrete measures obtained by the AIM and the PODAIM algorithm using the numerical realization of the Prohorov metric described in 5. In table 7.2 the Prohorov distances are listed after each algorithm has performed a multiple of the space dimension $N = 6$ and $l = 2$ respectively. The values indicate a convergence of the two discrete measures although a quite large distance remains until the end of the refinement process. This remainder is explained by the approximation error of the POD basis and can also be seen in the histogram where the shape of the higher-order fixed points differ.

m	$p(\mu_{mN}, \mu_{ml}^{[P]})$
1	0.2723
2	0.2342
3	0.1547
4	0.0794
5	0.0653
6	0.0872
7	0.0798
8	0.1170
9	0.0727
10	0.0824

Table 6: Prohorov distance of the discrete measures μ_k and $\mu_k^{[P]}$ computed by the AIM and PODAIM algorithm after mN and ml recursion steps

We end this section with a look to the result of the PODADAPT algorithm described in 6. With the same parameters as above we start with the AIM algorithm (in other words: $W = I_6$). The first computation of a new POD basis is performed after 12 recursion steps, i.e. after bisecting two times in each coordinate. Then, after every l recursion steps, which means one bisection in each coordinate, the POD basis is adapted and the state space is transformed. In Figure 5 we see the resulting histogram after 12 bisections in each coordinate. This corresponds to 47 recursion steps of the AIM algorithm, since the vector of POD dimensions occurring during the algorithm is

$$L = (6, 6, 6, 6, 6, 5, 2, 2, 2, 2, 2, 2)^T.$$

The Figure shows that the discrete measure approximates only the Dirac measures of the 2 stable fixed points. Other information about the system is apparently lost in the POD approximation process.

8 Outlook

This paper focusses on numerical aspects of computing invariant measures in high dimensional spaces. Several numerical as well as theoretical problems remain open. An important numerical goal is the improvement of the PODADAPT algorithm which is not yet very efficient.

The long-term theoretical goal is a convergence theory for the discrete measures computed by the PODAIM and PODADAPT algorithm respectively. This will require to generalize POD estimates that are well-known for single trajectories to the case of approximations when many short time trajectories. First promising results for easy systems have been established.

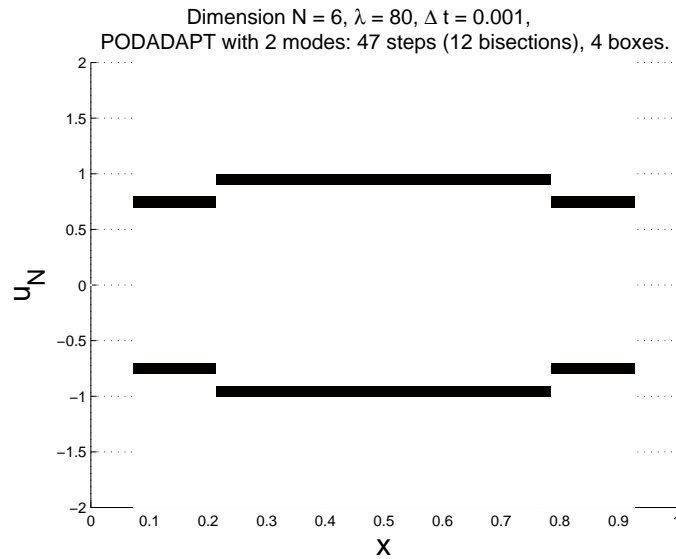


Figure 5: Resulting box collection of PODADAPT algorithm for the Chafee-Infante problem in $N = 6$ dimensions with parameter $\lambda = 80$. The current POD dimension after 12 bisections or $k = 47$ recursion steps is $l = 2$.

References

- [Ant05] A. C. Antoulas. *Approximation of large-scale dynamical systems*, Band 6 von *Advances in Design and Control*. Society for Industrial and Applied Mathematics (SIAM), Philadelphia, PA, 2005.
- [ASG01] A. C. Antoulas, D. C. Sorensen und S. Gugercin. A survey of model reduction methods for large-scale systems. In *Structured matrices in mathematics, computer science, and engineering, I (Boulder, CO, 1999)*, Band 280 von *Contemp. Math.*, Seiten 193–219. Amer. Math. Soc., 2001.
- [Bau92] H. Bauer. *Maß- und Integrationstheorie*. de Gruyter Lehrbuch. Walter de Gruyter & Co., Berlin, 2. Auflage, 1992.
- [Bil68] P. Billingsley. *Convergence of Probability Measures*. John Wiley & Sons Inc., New York, 1968.
- [CKR08] T. Caraballo, P. E. Kloeden und J. Real. Invariant measures and statistical solutions of the globally modified Navier-Stokes equations. *Discrete Contin. Dyn. Syst. Ser. B*, 10(4), Seiten 761–781, 2008.
- [DFJ01] M. Dellnitz, G. Froyland und O. Junge. The algorithms behind gaio - set oriented numerical methods for dynamical systems. *Ergodic Theory, analysis, and efficient simulation of dynamical systems*, 7, Seiten 145–174, 805–807, 2001.
- [DJ98] M. Dellnitz und O. Junge. An adaptive subdivision technique for the approximation of attractors and invariant measures. *Comput. Visual. Sci.*, 1, Seiten 63–68, 1998.
- [DJ99] M. Dellnitz und O. Junge. On the approximation of complicated dynamical behavior. *SIAM J. Numer. Anal.*, 36(2), Seiten 491–515, 1999.

- [Dud02] R. M. Dudley. *Real analysis and probability*, Band 74 von *Cambridge Studies in Advanced Mathematics*. Cambridge University Press, Cambridge, 2002.
- [GvL96] G. H. Golub und C. F. van Loan. *Matrix computations*. Johns Hopkins Studies in the Mathematical Sciences. Johns Hopkins University Press, Baltimore, 3. Auflage, 1996.
- [Hen81] D. Henry. *Geometric theory of semilinear parabolic equations*, Band 840 von *Lecture Notes in Mathematics*. Springer-Verlag, Berlin, 1981.
- [HLB96] P. Holmes, J. L. Lumley und G. Berkooz. *Turbulence, coherent structures, dynamical systems and symmetry*. Cambridge Monographs on Mechanics. Cambridge University Press, Cambridge, 1996.
- [JK] O. Junge und P. Koltai. Discretization of transfer operators using a sparse hierarchical tensor basis - the sparse ulam method. Preprint.
- [Jun01a] O. Junge. An adaptive subdivision technique for the approximation of attractors and invariant measures: Proof of convergence. *Dynamical Systems*, 16(3), Seiten 213–222, 2001.
- [Jun01b] O. Junge. Almost invariant sets in chua’s circuit. *Int. J. Bif. and Chaos*, 7, Seiten 2475–2485, 2001.
- [Kif86] Y. Kifer. General random perturbations of hyperbolic and expanding transformations. *J. Analyse Math.*, 47, Seiten 111–150, 1986.
- [KV01] K. Kunisch und S. Volkwein. Galerkin proper orthogonal decomposition methods for parabolic problems. *Numer. Math.*, 90(1), Seiten 117–148, 2001.
- [KV02] K. Kunisch und S. Volkwein. Galerkin proper orthogonal decomposition methods for a general equation in fluid dynamics. *SIAM J. Numer. Anal.*, 40(2), Seiten 492–515 (electronic), 2002.
- [Lar99] S. Larsson. Numerical analysis of semilinear parabolic problems. In *The graduate student’s guide to numerical analysis ’98 (Leicester)*, Band 26 von *Springer Ser. Comput. Math.*, Seiten 83–117. Springer, Berlin, 1999.
- [Lor63] E. Lorenz. Deterministic nonperiodic flow. *J. Atmos. Sci.*, 20, Seiten 130–141, 1963.
- [LSS94] S. Larsson und J. M. Sanz-Serna. The behavior of finite element solutions of semilinear parabolic problems near stationary points. *SIAM J. Numer. Anal.*, 31(4), Seiten 1000–1018, 1994.
- [LT03] S. Larsson und V. Thomée. *Partial differential equations with numerical methods*, Band 45 von *Texts in Applied Mathematics*. Springer-Verlag, Berlin, 2003.
- [MHvMD06] P. G. Mehta, M. Hessel-von Molo und M. Dellnitz. Symmetry of attractors and the Perron-Frobenius operator. *J. Difference Equ. Appl.*, 12(11), Seiten 1147–1178, 2006.
- [Min88] H. Minc. *Nonnegative matrices*. Wiley-Interscience Series in Discrete Mathematics and Optimization. John Wiley & Sons Inc., New York, 1988.
- [RCM04] C. Rowley, T. Colonius und R. Murray. Model reduction for compressible flows using pod and galerkin projection. *Physica D Nonlinear Phenomena*, 189(1-2), Seiten 115–129, 2004.
- [Rob01] J. C. Robinson. *Infinite-dimensional dynamical systems*. Cambridge Texts in Applied Mathematics. Cambridge University Press, Cambridge, 2001. An introduction to dissipative parabolic PDEs and the theory of global attractors.
- [Ula60] S. M. Ulam. *A collection of mathematical problems*. Interscience Tracts in Pure and Applied Mathematics, no. 8. Interscience Publishers, New York-London, 1960.