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CONVERGENCE RATES OF THE POD–GREEDY METHOD

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Abstract. Iterative approximation algorithms are successfully applied in parametric approximation tasks. In particular, reduced basis methods make use of the so-called Greedy algorithm for approximating solution sets of parametrized partial differential equations. Recently, *a priori* convergence rate statements for this algorithm have been given (Buffa *et al.* 2009, Binev *et al.* 2010). The goal of the current study is the extension to time-dependent problems, which are typically approximated using the POD–Greedy algorithm (Haasdonk and Ohlberger 2008). In this algorithm, each greedy step is invoking a temporal compression step by performing a proper orthogonal decomposition (POD). Using a suitable coefficient representation of the POD–Greedy algorithm, we show that the existing convergence rate results of the Greedy algorithm can be extended. In particular, exponential or algebraic convergence rates of the Kolmogorov n-widths are maintained by the POD–Greedy algorithm.

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1. Introduction

The goal of low dimensional approximation of function sets is becoming increasingly important as indicated by the growing efforts in the field of model order reduction (MOR) for stationary or dynamical systems. In particular, solution sets of parametrized partial differential equations are one of the central objects in reduced basis (RB) methods. These assume a compact parameter set $\mathcal{P} \subset \mathbb{R}^p$ and a parametrized partial differential equation (PDE), whose solutions $u(\mu)$ for $\mu \in \mathcal{P}$ form a (at most) p-dimensional manifold in a solution space X. RB-methods identify compact linear subspaces $X_N \subset \operatorname{span}(u(\boldsymbol{\mu}^1), \ldots, u(\boldsymbol{\mu}^n)))$ constructed by particular solutions $u(\boldsymbol{\mu}^i) \in X$, the so-called *snapshots*. We refer to [18] and references therein for a general overview over this class of methods. The crucial questions is, how to choose the parameter samples $(\boldsymbol{\mu}^i)_{i=1}^n$ in order to obtain a reduced space that allows to approximate the solution manifold well. For simple problems, *e.g.* one-parameter elliptic coercive problems, it has been shown that a logarithmically equidistant choice of snapshot parameters yields exponential convergence of the approximation error [16]. Such analytical results however only existed for rather simple cases. For general problems, where no *a priori* information about the structure of the manifold exists, one refrains to practical algorithms that result in good convergence rates. The so-called Greedy algorithm, introduced in the context of RB-methods in [22], has developed to be the method-of-choice for stationary PDEs. This method is an incremental constructive method for basis generation. Starting with a small initial basis, the

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parameter for the currently worst resolved solution is identified by a search over (a fine but finite subset of) the parameter domain. The solution for this worst parameter is computed and used as next basis element. These search and extension steps are repeated until a sufficiently high accuracy of the reduced basis is obtained. The accuracy and error in this procedure needs to be evaluated multiple times and hence is typically not computed exactly, but evaluated by means of rapidly computable rigorous and effective *a-posteriori* error bounds. Only recently, efforts have been started to get formal foundation for this primary heuristic algorithm. The central concept for approximability of sets by linear subspaces is the so-called Kolmogorov n-width. Intuitively, the Kolmogorov n-width is the worst approximation error of the best n-dimensional subspace. Explicit bounds for these n-widths are known for certain compact sets [10], function classes such as Sobolev balls [20] or solution sets of differential operators [17]. This approximation theoretic concept has been successfully applied to explain the success of the Greedy algorithm. In particular, it has recently been shown that possible exponential convergence rate of the Kolmogorov n-width transfers to the approximation error of the Greedy algorithm [2]. These results have been refined and extended to the case of algebraic convergence [1]. The latter will be the most important reference for the current study, as we will extend those results.

Our extension concerns the treatment of time-dependent RB-methods. In the time-discrete formulation, a single solution consists of a sequence of possibly several hundred snapshots over time. Hence, an inclusion of all snapshots along a trajectory during basis-enrichment is not feasible. Nor, a selection of single snapshots from the sequence seems suitable, as a stalling of the basis-enrichment can be observed [5]. As a practical and well-performing alternative, we suggested and introduced the POD–Greedy algorithm in our work [6]. This algorithm is a combination of the Greedy algorithm with a temporal compression step.

The crucial ingredient for time-sequence compression is the use of a principal component analysis (PCA) [3,11] of the snapshots' Grammian matrix. Different notions for this method can be found in different research fields. In probability theory it was introduced as Karhunen–Loeve transformation [12, 15], or even earlier in statistics as Hotelling transformation [9]. In the field of numerical analysis for partial differential equations and model order reduction, the notion proper orthogonal decomposition (POD) is very common. Therefore, we adopt this terminology. Important fields of application of the POD are parabolic partial differential equations [14] or problems in fluid dynamics [8]. A good motivation for using low-dimensional models, such as obtained from POD, are sophisticated simulation scenarios such as optimal control [7].

The POD–Greedy method for reduced basis construction meanwhile has developed to the standard procedure for instationary problems [4, 6, 13]. Still, it lacks theoretical foundation, and hence is only a heuristic method so far. In the current paper, we will extend the convergence results of the Greedy algorithm for stationary problems [1] to the POD–Greedy algorithm for time-dependent (or more general: sequence-based) problems. We will similarly show that exponential or algebraic convergence rates of the Kolmogorov n-width of the to be approximated set are maintained by the POD–Greedy algorithm only by a change of the multiplicative factor and the exponent.

The paper is structured as follows. In the next section, we provide the basic notation and definitions of the functional setting and approximability measures. Section 3 gives the definition of the POD, the POD–Greedy algorithm and derives several formal properties that are required for the convergence analysis. In Section 4 we prove the main lemma for obtaining the subsequent convergence rate estimates. We conclude in Section 5 with some comments on future work.

2. Basic notation

Let X be a separable real Hilbert space with corresponding scalar product $\langle \cdot, \cdot \rangle$ and norm $\| \cdot \|$. Let $0 \leq t^0 < \ldots < t^K \leq T$ be $K+1$ time-instants on the finite time interval $[0, T]$ and set $\mathbb{T} := \{t^k\}_{k=0}^K$. Here and in the following we make use of the convention that superscripts k do not indicate powers, but time-indices. Let $X_T := L^2(\mathbb{T}, X)$ denote the space of time-sequences of elements stemming from X. For $u \in X_T$ we abbreviate $u^k := u(t^k) \in X$. X_T is endowed with a (weighted) L^2-scalar product $\langle u, v \rangle_T := \sum_{k=0}^K w^k u^k v^k$ with suitable weights $w^k \in \mathbb{R}^+ \backslash \{0\}$ satisfying $\sum_{k=0}^K w^k = T$. The corresponding induced norm is denoted with $\|\cdot\|_T$. We introduce the diagonal matrix $W := \text{diag}(w^0, \dots, w^K) \in \mathbb{R}^{(K+1)\times(K+1)}$ and define a norm on $\mathbb{R}^{K+1}$ by $\|v\|_W := \sqrt{v^T W v}, v \in \mathbb{R}^{K+1}$. Typical choices for w^k comprise $w^k = T/(K+1)$ for piecewise midpoint integration or $w^0 = w^K = T/(2K), w^k = T/K, 0 < k < K$ for the piecewise trapezoidal quadrature rule. In the argumentation, the specific values of w^k will be of minor importance, so the reader can safely think of $w^k = 1$. But we want to cover the general setting and obtain the dependence of the final constants on K, T, so we carry these weights w^k through the argumentation. We assume the goal of approximating a compact set (of sequences) $\mathcal{F}_T \subset X_T$. The approximation will not be obtained *via* arbitrary subspaces of X_T but *via* spaces constructed by *flat* approximating spaces. More precisely: In addition to $\mathcal{F}_T$ we introduce $\mathcal{F} := \{u(t^k) | u \in \mathcal{F}_T, k = 0, \dots, K\} \subset X$ as the *flat* set. The elements $u(t^k)$ will be denoted *snapshots* of the solution trajectory $u \in \mathcal{F}_T$. The flat set $\mathcal{F}$ is compact in X as it is the union of $K+1$ compact sets *via* the component projections. We assume finite dimensional flat spaces $X_n \subset \text{span}(\mathcal{F}) \subset X$, $\dim(X_n) = n, n \in \mathbb{N}_0$ and define the approximating spaces of sequences $X_{T,n} \subset X_T$ by

$$X_{T,n} := L^2(\mathbb{T}, X_n) \subset X_T. \tag{2.1}$$

We emphasize that in contrast to the time-independent case, the spaces X_n are not directly subspaces spanned by snapshots. As a POD will be involved, the spaces will be given as *subspaces* of the span of certain snapshots. Note, that for finite $\mathcal{F}_T$ the space dimension will be bounded by $n \leq |\mathcal{F}_T| \cdot (K+1)$, but in general $\mathcal{F}_T$ is assumed to be infinite, allowing arbitrarily large n. For the flat subspaces X_n we introduce the orthogonal projection operators $P_n : X \to X_n$. For the approximating sequence spaces $X_{T,n}$ we analogously define $P_{T,n}$. Note that due to our choice of sequence spaces the sequence best-approximation is equivalent to componentwise best-approximation and hence $(P_{T,n}(u))^k = P_n(u^k)$ for all $u \in \mathcal{F}_T$, $k = 0, \dots, K$.

The relevant quantity of approximability is the Kolmogorov n-width of the flat set $\mathcal{F}$ in X:

$$d_n := d_n(\mathcal{F}) := \inf_{\substack{Y \subset X \\ \dim(Y) = n}} \sup_{f \in \mathcal{F}} \inf_{\hat{f} \in Y} \|f - \hat{f}\|, \quad n \geq 0. \tag{2.2}$$

Alternatively, one might be tempted to consider the Kolmogorov n-width of the time-sequence set $\mathcal{F}_T$ in X_T, $d_n(\mathcal{F}_T)$. This, however, is not adequate in our context: In view of (2.1) we do not consider arbitrary subspaces of $\mathcal{F}_T$, but only spaces defined by the identical flat space at each time-instant. Further, for the approximating sequence spaces we would have $\dim(X_{T,n}) = n(K+1)$, hence n-dimensional approximating sequence subspaces would not have relevance.

The error measure which is relevant for the POD–Greedy is the maximum (weighted) L^2 approximation error of the sequence set $\mathcal{F}_T$, *i.e.* for $n \geq 0$

$$\sigma_{T,n} := \sigma_{T,n}(\mathcal{F}_T) := \sup_{u \in \mathcal{F}_T} \|u - P_{T,n} u\|_T = \sup_{u \in \mathcal{F}_T} \sqrt{\sum_{k=0}^{K} w^k \|u^k - P_n u^k\|^2}. \tag{2.3}$$

Again, other spaces may seem possible candidates for the definition of the approximation error, *e.g.* the approximation error for the flat space X, or other variants, but they turn out to be of minor importance in the analysis.

We give a few comments on realization of the above choices in RB-methods for time-dependent problems: The flat solution space is frequently a Hilbert space of real valued functions on a bounded domain $\Omega \subset \mathbb{R}^d$, *e.g.* $X = L^2(\Omega)$ or $X = H_0^1(\Omega)$, hence separable. After suitable time-discretization, a numerical scheme produces a solution trajectory $u = (u^k)_{k=0}^K \in X_T$. A compact parameter set $\mathcal{P} \subset \mathbb{R}^p$ is given and the solution of the parametrized problem $u(\boldsymbol{\mu}) \in X_T$ is assumed to be well defined and to have a continuous parameter dependence. This guarantees the compactness of the set $\mathcal{F}_T := \{u(\boldsymbol{\mu}) | \boldsymbol{\mu} \in \mathcal{P}\} \subset X_T$ as required above.

Remark 2.1 (Generalization to further sequence-based schemes)**.**

We deliberately choose a discrete-in-time rather than a time-continuous formulation, as this is the only way in which the algorithm currently is applied. However, we do not exclude that a time-continuous formulation and investigation would similarly be possible. By the time-discrete formulation, however, we are not limited to instationary PDEs, but can treat any scenario where a solution consists of a sequence of functions. For instance, the above framework also comprises nonlinear stationary problems, where k plays the role of a Newton-iteration number, K being a globally fixed number of Newton iterations. Further, also iterative domain decomposition schemes are covered by the formalization, where k is the iteration number and K is a globally fixed number of iterations for accepting the final solution. The set of time-instants $\mathbb{T}$ is then merely an abstract index set without interpretation as time.

3. Abstract POD–Greedy algorithm

For a given function sequence $u \in X_T$, we introduce the (scaled) empirical correlation operator $R : X \to X$ defined as

$$R(v) := \sum_{k=0}^{K} w^k \left\langle u^k, v \right\rangle u^k, \quad v \in X. \tag{3.1}$$

This operator is linear, continuous, positive semidefinite, self-adjoint, and has a finite dimensional range $R(X) = \mathrm{span}\{u^k\}_{k=0}^K$, hence is compact. Due to the spectral theorem, for $u \neq 0$ it has a discrete finite spectrum of $L+1$ eigenvalues $\{\lambda_k\}_{k=0}^L \subset \mathbb{R}^+ \backslash \{0\}$ for some $0 \leq L \leq K$ with corresponding orthonormal eigenfunctions $\{\varphi_k\}_{k=0}^L \subset \mathrm{span}\{u^k\}_{k=0}^K$ such that

$$R(v) = \sum_{k=0}^{L} \lambda_k \left\langle \varphi_k, v \right\rangle \varphi_k, \tag{3.2}$$

where we assume descending eigenvalues, $\lambda_i \geq \lambda_j$ for $i < j$. To emphasize the dependence on $u \in X_T$, we occasionally write $\lambda_i(u)$. Note that the eigenvalues also depend on the chosen time grid $\{t^k\}_{k=0}^K$. For $0 \leq l \leq L$ we define the POD–basis as $POD_l : X_T \to X^l$ (l here indicating a cartesian product power $X^l := \times_{i=1}^{l} X$) by

$$POD_l(u) := (\varphi_0, \ldots, \varphi_{l-1}) \in X^l.$$

Note that due to the possible non-uniqueness of normalized eigenfunctions, this operation could be seen as being set-valued. In practice, an arbitrary ensemble of eigenfunctions is chosen.

This orthonormal POD–basis satisfies a best-approximation property

$$\mathrm{span}(POD_l(u)) \in \arg \min_{\substack{Y \subset X \\ \dim(Y)=l}} \sum_{k=0}^{K} w^k \|u^k - P_Y u^k\|^2. \tag{3.3}$$

The eigenvalue problem for R is high or even infinite dimensional, and can be recast as a $K+1$-dimensional problem *via* the Gramian matrix of the snapshots. The corresponding eigenvectors of the Grammian then represent the coefficient vectors of the corresponding eigenfunctions of R in the span of the snapshots. Correspondingly, this procedure is sometimes called the *method of snapshots* [19]. A practical recipe for the computation of the eigenvalue problem in our weighted setting can then be summarized as follows. Similar detailed analysis can be found in [23].

Lemma 3.1 (POD *via* Kernel matrix)**.**

We introduce the Kernel (or Gramian) matrix $G := \left(\left\langle u^i, u^j \right\rangle\right)_{i,j=0}^K \in \mathbb{R}^{(K+1)\times(K+1)}$ *and its weighted version* $\tilde{G} = WG$*. Let* $\tilde{V}\tilde{\Lambda}\tilde{V}^{-1} = \tilde{G}$ *be an eigenvalue decomposition with eigenvalues* $\tilde{\Lambda} = \mathrm{diag}(\tilde{\lambda}_0, \ldots \tilde{\lambda}_K)$ *monotonically* *decreasing and eigenvectors* $\tilde{V} = (\tilde{v}_0, \dots, \tilde{v}_K)$, *which are assumed to be scaled such that* $\tilde{v}_i^T G \tilde{v}_i = 1$ *if* $\tilde{\lambda}_i \neq 0$. *Then for all* i *with* $\tilde{\lambda}_i \neq 0$, $\tilde{\lambda}_i$ *is also an eigenvalue of* R *with unit length eigenvector*

$$\varphi_i = \sum_{k=0}^{K} (\tilde{v}_i)_k u^k, \tag{3.4}$$

where $\tilde{v}_i = ((\tilde{v}_i)_k)_{k=0}^K \in \mathbb{R}^{K+1}$.

Proof. From the definition of the correlation operator we see that $(\varphi_i, \tilde{\lambda}_i)$ is an eigenvector/-value pair:

$$R\left(\sum_{k=0}^{K} (\tilde{v}_i)_k u^k\right) = \sum_{k,k'=0}^{K} u^{k'} w^{k'} \left\langle u^{k'}, u^k \right\rangle (\tilde{v}_i)_k = \sum_{k'=0}^{K} u^{k'} \left(WG\tilde{v}_i\right)_{k'} = \tilde{\lambda}_i \sum_{k'=0}^{K} u^{k'} (\tilde{v}_i)_{k'}.$$

Unit scaling of φ_i is verified by

$$\|\varphi_i\|^2 = \sum_{k,k'} (\tilde{v}_i)_k (\tilde{v}_i)_{k'} \left\langle u^k, u^{k'} \right\rangle = \tilde{v}_i^T G \tilde{v}_i = 1. \qquad \square$$

For further details on the POD resp. PCA, we refer to [11, 23].

Given the notation above, the POD–Greedy algorithm can be formulated in an abstract way. For simplicity of presentation, we only consider the case $l = 1$, *i.e.* only include a single POD–mode in each iteration. We give a *weak* formulation similar to [1], which means that maximization operations are allowed to deviate from the real maximum by a certain prescribed factor $\gamma \in (0, 1]$.

Definition 3.2 (Weak POD–Greedy algorithm)**.**

1. Define $X_0 := \{0\} \subset X$ and $X_{T,0} := L^2(\mathbb{T}, X_0) \subset X_T$.
2. For $n \in \mathbb{N}$
   2a. choose $u_n \in \mathcal{F}_T$ such that

$$\|u_n - P_{T,n-1} u_n\|_T \geq \gamma \max_{u \in \mathcal{F}_T} \|u - P_{T,n-1} u\|_T. \tag{3.5}$$

   2b. Compute $f_n = \mathrm{POD}_1(u_n - P_{T,n-1} u_n) \in X$.
   2c. Define $X_n := X_{n-1} \oplus \mathrm{span}(f_n)$ and $X_{T,n} := L^2(\mathbb{T}, X_n)$.

In practice, the algorithm is assigned a stopping criterion such as an error threshold or a maximum number of basis functions to generate. As we are interested in asymptotic convergence rates, we assume that the above sequence always results in $u_n - P_{T,n-1} u_n \neq 0$, otherwise we have obtained exact approximation after finitely many steps.

The factor γ accomplishes for equivalence factors between the projection error and RB *a-posteriori* error estimators which are used as rapidly computable substitutes: If an error estimator $\Delta(u)$ satisfies $c\Delta(u) \leq \|u - P_{T,n} u\|_T \leq C\Delta(u)$ for any $u \in \mathcal{F}_T$, then maximizing $\Delta(u)$ will at least reach the $\frac{c}{C}$ fraction of the true maximal projection error, hence $\gamma := \frac{c}{C}$ is a suitable choice in the abstract algorithm. Such RB error estimators can be obtained for PDE discretizations, which can be recast in an inf-sup stable space-time Petrov–Galerkin formulation. For example, parabolic problem such as the heat-equation, but as well convection-dominant conservation laws can be treated [6, 21].

We state some simple properties of the POD and POD–Greedy algorithm that will be used in the convergence analysis:

Lemma 3.3 (Properties of the POD/POD–Greedy)**.**

i) For all $u \in X_T$ the POD–eigenvalues satisfy

$$\sum_{k=0}^{K} \lambda_k(u) = \|u\|_T^2. \tag{3.6}$$

ii) The resulting family of functions $(f_n)_{n\in\mathbb{N}}$ is orthonormal, $\langle f_n, f_m\rangle = \delta_{nm}$.

Proof.

i) Setting $u^k = \sum_{k'=0}^{K} c_{k'}^k \varphi_{k'}$ for suitable $c_{k'}^k \in \mathbb{R}$, the definition of R in (3.1) and orthonormality of $\{\varphi_k\}$ gives

$$\langle R(\varphi_{k'}), \varphi_{k'}\rangle = \left\langle \sum_{k=0}^{K} w^k \left\langle u^k, \varphi_{k'} \right\rangle u^k, \varphi_{k'} \right\rangle = \sum_{k=0}^{K} w^k \left\langle u^k, \varphi_{k'} \right\rangle^2 = \sum_{k=0}^{K} w^k (c_{k'}^k)^2.$$

Additionally, we have $\|u^k\|^2 = \sum_{k'=0}^{K} (c_{k'}^k)^2$ and conclude with the spectral decomposition (3.2)

$$\sum_{k'=0}^{K} \lambda_{k'} = \sum_{k'=0}^{K} \langle R(\varphi_{k'}), \varphi_{k'}\rangle = \sum_{k,k'=0}^{K} w^k (c_{k'}^k)^2 = \sum_{k=0}^{K} w^k \|u^k\|^2 = \|u\|_T^2.$$

ii) The range of the correlation operator R in (3.1) is the span of the training samples, *i.e.* $f_n \in \mathrm{span}\{u_n^k - P_{n-1}u_n^k\}_{k=0}^K$. The orthogonality of the projection error implies $f_n \perp X_{n-1}$, which yields the statement by induction. □

At this point it is simple to show the convergence of the POD–Greedy method.

Proposition 3.4 (Convergence of the POD–Greedy)**.**
The sequence of approximation errors $\sigma_{T,n}$ defined by (2.3) is monotonically decreasing, $\sigma_{T,n} \geq \sigma_{T,m}$ for $n \leq m$ and $\lim_{n\to\infty} \sigma_{T,n} = 0$.

Proof. The orthogonal projection yields a best-approximation and for $n \leq m$ we have $X_n \subset X_m$, hence

$$\|u^k - P_n u^k\| = \inf_{f \in X_n} \|u^k - f\| \geq \inf_{f\in X_m} \|u^k - f\| = \|u^k - P_m u^k\|$$

and the monotonicity statement follows in view of (2.3). As a consequence, the sequence $(\sigma_{T,n})_{n\in\mathbb{N}}$ converges to a nonnegative limit, $\sigma^* := \lim_{n\to\infty} \sigma_{T,n} \geq 0$. Assuming $\sigma^* > 0$ then leads to a contradiction: Choose arbitrary $m > n \in \mathbb{N}$ and consider the corresponding two elements of the sequence of selected trajectories, these satisfy

$$\|u_m - u_n\|_T \geq \|u_m - P_{T,n}u_m\|_T \geq \|u_m - P_{T,m-1}u_m\|_T \geq \gamma \sup_{u\in\mathcal{F}_T} \|u - P_{T,m-1}u\|_T = \gamma\sigma_{T,m-1} \geq \gamma\sigma^*.$$

Obviously $(u_n)_{n\in\mathbb{N}}$ does not have a converging subsequence contradicting the compactness of $\mathcal{F}_T$. Therefore, we conclude that $\sigma^* = 0$. □

We comment on two extreme cases concerning the eigenvalue spectrum. These cases can appear in practice and both are to be covered by the subsequent analysis.

Example 3.5 (Worst/Best case advection problem)**.** Consider the (non-parametric) advection problem $\partial_t\psi + \partial_x\psi = 0$ on $\Omega = [0, K+1], T = K$ and set $t^k := k$ and $x_k := k$ for $k = 0, \ldots K$. Assume initial data $\psi = \psi_0$ with $\psi_0(x_k) = \delta_{0k}$ being piecewise linear on all intervals $[k, k+1]$ and cyclical boundary conditions. Set $X = \mathbb{R}^{K+1}, w^k := 1$. Then an (*e.g.* upwind finite difference) discretization yields $u = (u^k)_{k=0}^K$ with $u^k = (\delta_{ki})_{i=0}^K$ discretizing the solution $(u^k)_i = \psi(t^k, x_i)$. The set $\mathcal{F}_T := \{u\} \subset X_T$ contains a single trajectory. Obviously, u^k are already orthonormal, hence the correlation operator R in (3.1) is already in spectral form with eigenvalues $\lambda_0 = \ldots = \lambda_L = 1$ and $L = K$. Hence, here indeed in each step of the POD–Greedy algorithm one single mode is inserted decreasing the error $\sigma_{T,n}^2$ by an identical decrement. This is the worst case example of no decay in the eigenvalue spectrum. The convergence rate proof respects this worst case. On the contrary, consider $\partial_t u = 0$ as stationary (but time-dependent) problem with identical initial and boundary data as before. Then $u^k = (1, 0, \ldots, 0)^T \in \mathbb{R}^{K+1}$ are identical for all k. The correlation operator has a single nonzero eigenvalue $\lambda_0 = K + 1$ with eigenfunction $\varphi_0 = u^1$. Inserting one mode of the POD yields exact approximation of the trajectory. This is the best case of an eigenvalue spectrum with one nonzero eigenvalue, *i.e.* $L = 0$.

3.1. A coefficient representation of the POD–Greedy

The crucial point in the convergence analysis is the specification of a coefficient representation of the algorithm and proofs of some of the characterizing coefficient properties.

The POD–Greedy algorithm generates a sequence of trajectories $u_j \in \mathcal{F}_T$ and orthonormal functions $f_j \in X$. For $i, j \in \mathbb{N}$ we then can define vectors $a_{ij} \in \mathbb{R}^{K+1}$ by

$$(a_{ij})_k := \left\langle u_i^k, f_j \right\rangle, \quad k = 0, \ldots K.$$

If $u_n = u_{n'}$, *i.e.* a sequence is selected at POD–Greedy-iteration n and n', then also $a_{nj} = a_{n'j}, j \in \mathbb{N}$, hence they are indiscriminable. Clearly, any sequence u_n can only be selected $K + 1$ times due to definition of the POD–Greedy algorithm.

We state some properties of the coefficient vectors that will be required later.

Proposition 3.6 (Properties of POD–Greedy coefficient vectors)**.**

i) For all $n \in \mathbb{N}$ we have

$$\sum_{j\in\mathbb{N}} \|a_{nj}\|_W^2 = \|u_n\|_T^2.$$

ii) For all $i, n \in \mathbb{N}$ we have

$$\sum_{j\geq n} \|a_{ij}\|_W^2 = \|u_i - P_{T,n-1}u_i\|_T^2,$$

hence in particular, if $u_i - P_{T,n-1}u_i = 0$, then $a_{ij} = 0 \in \mathbb{R}^{K+1}$ for all $j \geq n$.

iii) For all $n \in \mathbb{N}$ we have

$$\|a_{nn}\|_W \geq \|a_{nj}\|_W, \quad j \geq n.$$

iv) For all $n \in \mathbb{N}$ we have

$$\|a_{nn}\|_W^2 = \lambda_0(u_n - P_{T,n}u_n) \geq \gamma^2\sigma_{T,n}^2/(K+1).$$

v) For all $i, n \in \mathbb{N}$ with $u_n = u_i$ we have

$$\gamma^2\sigma_{T,n}^2 \leq \sum_{j\geq n} \|a_{ij}\|_W^2 \leq \sigma_{T,n}^2.$$

The right inequality also holds if $u_n \neq u_i$.

Proof.

i) The convergence statement in Proposition 3.4 implies that $0 = \lim_{m\to\infty} \|u - P_{T,m}u\|_T^2$ for all $u \in \mathcal{F}_T$. Then $u = \lim_{m\to\infty} P_{T,m}u$ which implies for each slice $u^k = \lim_{m\to\infty} P_m u^k$. As $(f_j)_{j\in\mathbb{N}}$ is an orthonormal family we get for each u_n^k from the POD–Greedy selected trajectories

$$u_n^k = \lim_{m\to\infty} P_m u_n^k = \lim_{m\to\infty} \sum_{j=0}^{m} \left\langle u_n^k, f_j \right\rangle f_j = \sum_{j\in\mathbb{N}} (a_{nj})_k f_j,$$

hence $\|u_n^k\|^2 = \sum_{j\in\mathbb{N}} ((a_{nj})_k)^2$ and

$$\|u_n\|_T^2 = \sum_{k=0}^{K} w^k \|u_n^k\|^2 = \sum_{k=0}^{K} w^k \sum_{j\in\mathbb{N}} ((a_{nj})_k)^2 = \sum_{j\in\mathbb{N}} \|a_{nj}\|_W^2 \,.$$

ii) We note that

$$\|P_{n-1}u_i^k\|^2 = \|\sum_{j=1}^{n-1} \left\langle u_i^k, f_j \right\rangle f_j\|^2 = \sum_{j=1}^{n-1} \left\langle u_i^k, f_j \right\rangle^2 = \sum_{j=1}^{n-1} ((a_{ij})_k)^2.$$

Then we get

$$\|P_{T,n-1}u_i\|_T^2 = \sum_{k=0}^{K} w^k \|P_{n-1}u_i^k\|^2 = \sum_{j=1}^{n-1} \|a_{ij}\|_W^2 \,.$$

The claim then follows from the Pythagorean theorem with i).

iii) For any $u^k, f \in X$ with $\|f\| = 1$ we verify

$$\|u^k - \left\langle u^k, f \right\rangle f\|^2 = \left\langle u^k, u^k \right\rangle - 2\left\langle u^k, f \right\rangle^2 + \left\langle u^k, f \right\rangle^2 \left\langle f, f \right\rangle = \left\langle u^k, u^k \right\rangle - \left\langle u^k, f \right\rangle^2 .$$

This can be used to rewrite the POD-optimality property (3.3) as a maximization over f:

$$f_n \in \arg\min_{\|f\|=1} \sum_{k=0}^{K} w^k \|u_n^k - \left\langle u_n^k, f \right\rangle f\|^2 = \arg\max_{\|f\|=1} \sum_{k=0}^{K} w^k \left\langle u_n^k, f \right\rangle^2 .$$

This implies for all $j \geq n$

$$\|a_{nn}\|_W^2 = \sum_{k=0}^{K} w^k \left\langle u_n^k, f_n \right\rangle^2 \geq \sum_{k=0}^{K} w^k \left\langle u_n^k, f_j \right\rangle^2 = \|a_{nj}\|_W^2 \,.$$

iv) The right inequality follows from using $\lambda_0(u) \geq \lambda_k(u)$ for all $u \in X_T$, (3.6), the weak optimality of the greedy selection rule (3.5) and the definition of $\sigma_{T,n}$ (2.3):

$$(K+1)\lambda_0(u_n - P_{T,n}u_n) \geq \sum_{k=0}^{K} \lambda_k(u_n - P_{T,n}u_n) = \|u_n - P_{T,n-1}u_n\|_T^2 \geq \gamma^2 \sigma_{T,n}^2.$$

The left equality follows from the definition (3.1) and decomposition (3.2) of R

$$\begin{aligned}\|a_{nn}\|_W^2 &= \sum_{k=0}^{K} w^k ((a_{nn})_k)^2 = \sum_{k=0}^{K} w^k \left\langle u_n^k, \varphi_0 \right\rangle^2 \\ &= \left\langle \sum_{k=0}^{K} w^k \left\langle u_n^k, \varphi_0 \right\rangle u_n^k, \varphi_0 \right\rangle = \left\langle R(\varphi_0), \varphi_0 \right\rangle = \lambda_0.\end{aligned}$$

v) From the weak-POD–Greedy selection property (3.5) and definition of $\sigma_{T,n}$ (2.3) we get

$$\gamma^2 \sigma_{T,n}^2 \leq \|u_n - P_{T,n-1} u_n\|_T^2 \leq \sigma_{T,n}^2,$$

which exactly is the statement in view of ii) for $u_n = u_i$. If $u_n \neq u_i$ then still the right inequality holds. □

Remark 3.7 (Interpretation as isometric embedding into $(l^2(\mathbb{N}))^{K+1}$)**.** We consider $\bar{X} := l^2(\mathbb{N})^{K+1}$ with elements $(a_k)_{k=0}^K \in \bar{X}, a_k \in l^2(\mathbb{N})$ which is a separable Hilbert space with respect to the weighted inner product

$$\langle (a_k), (a'_k) \rangle_{\bar{X}} := \sum_{k=0}^{K} w^k \langle a_k, a'_k \rangle_{l^2} .$$

Let $u_n \in \mathcal{F}_T$ be selected by the POD–Greedy algorithm at iteration n with corresponding coefficient vectors $a_{nj} \in \mathbb{R}^{K+1}, j \in \mathbb{N}$. Then

$$J : \{u_n\}_{n\in\mathbb{N}} \to \bar{X}, J(u_n) := ((a_{nj}))_{j\in\mathbb{N}} \tag{3.7}$$

is an isometric embedding.

Intuitively, this situation can be visualized as follows. All u_n^k can be expressed as linear combination of the $\{f_j\}$ by (3.1). We write this as an infinite matrix-vector-multiplication using the vectors $a_{nj} \in \mathbb{R}^{K+1}$ as matrix blocks:

$$\left(\begin{array}{c} u_1^0 \\ \vdots \\ u_1^K \\ \hline u_2^0 \\ \vdots \\ u_2^K \\ \hline \vdots \end{array}\right) = \left(\begin{array}{c|c|c|c} a_{11} & a_{12} & a_{13} & \dots \\ \hline a_{21} & a_{22} & a_{23} & \dots \\ \hline \vdots & \vdots & \vdots & \ddots \end{array}\right) \begin{pmatrix} f_1 \\ f_2 \\ f_3 \\ \vdots \end{pmatrix} \tag{3.8}$$

Equation (3.7) implies that $J(u_n)$ is the n-th (block)–row of this matrix which has an infinite number of columns. The POD–Greedy applied to $\tilde{\mathcal{F}}_T := J(\mathcal{F}_T)$ will have $(\tilde{u}_n)_{n\in\mathbb{N}} := (J(u_n))_{n\in\mathbb{N}}$ as a possible sequence of selected trajectories and generated unit basis vectors $\tilde{f}_n = e_n \in l^2(\mathbb{N})$.

In contrast to the Greedy case of [1], the coefficients cannot simply be arranged as a lower-triangular matrix, but the matrix has block structure and is more dense. This is due to the fact that in the POD–Greedy algorithm one trajectory can possibly be chosen multiple times, because a single selection and basis enrichment does not guarantee zero error. Several properties stated in the previous propositions can be translated into corresponding matrix properties. For example, there may be up to $K+1$ block–rows, which are identical, indicating a multiple selection of one sequence. It may happen that a block-row does not contain any zero-vectors indicating that no precise approximation by finite subspaces is reached. On the contrary, any case of finite exact approximation, $u_n - P_{T,n-1}u_n = 0$, is reflected in the matrix as $a_{nj} = 0, j \geq n$ by Proposition 3.6 ii). In the case of $K = 0$, we recover the Greedy–algorithm, the vectors a_{ij} reduce to scalars and the matrix is lower triangular as in [1].

4. Convergence rates

Based on the findings from the previous sections, the arguments of [1] for obtaining convergence rate statements can be adopted.

4.1. Control of the approximation error sequence

The central step for obtaining convergence rate statements for the Greedy algorithm is the control of the approximation error sequence by the Kolmogorov n-width sequence. In our case, the *flatness lemma* [1], Lemma 2.2 can be extended for the POD–Greedy algorithm. It states that if the error sequence of the POD–Greedy scheme is not decaying too fast (being *flat*), then the Kolmogov n-width at a certain iteration number must be large. This is also denoted *delayed comparison* lemma, as $\sigma_{T,n}$ and d_m are compared with different indices n, m.

Lemma 4.1 (Flatness lemma for the POD–Greedy algorithm)**.** *Let* $\theta \in (0,1)$ *be given and* $q \in \mathbb{N}$ *with* $q = \lceil (2\gamma^{-1}\theta^{-1}\sqrt{K+1}\rceil^2$. *If* $n, m \in \mathbb{N}$ *are such that*

$$\sigma_{T,n+qm} \geq \theta\sigma_{T,n} \tag{4.1}$$

then we have

$$\sigma_{T,n} \leq \sqrt{qT}d_m. \tag{4.2}$$

Before providing the proof, we comment on the two notable extensions compared to [1], Lemma 2.2 and argue, why these in general can not be eliminated.

Remark 4.2.

i) The final estimate (4.2) has an additional factor $\sqrt{T}$ compared to the case of the Greedy algorithm. This is expected due to the fact that we are comparing the approximability properties of the flat set (quantified by d_m) with an approximation error of time-sequences measured in the X_T norm. Therefore, the $\sqrt{T}$ factor is suitable.
ii) The constant q (and herewith also the final bound) depends on a factor $K+1$ which essentially indicates a dependency on the number of time-steps. This is due to the fact that the proof respects the worst case scenario, *i.e.* all eigenvalues of R being identical and the overall error decrease in every POD–Greedy step only being $\sigma_n^2/(K+1)$. This is realistic in transport problems of discontinuous functions, see Example 3.5. By additional assumptions on the decay rate of the eigenvalues, this might be reformulated. As we are mainly interested in convergence rates, we are content with the current factors.

Proof of Lemma 4.1. Set $\bar{n} = n + qm$ and consider the block matrix

$$G = \begin{pmatrix} a_{nn} & \dots & a_{n\bar{n}} \\ \vdots & & \vdots \\ a_{\bar{n}n} & \dots & a_{\bar{n}\bar{n}} \end{pmatrix} \in \mathbb{R}^{(K+1)(1+qm)\times(1+qm)}.$$

We define

$$g_i^k := \sum_{j=n}^{\bar{n}} (a_{ij})_k f_j \in X, i = n, \dots \bar{n}, k = 0, \dots K$$

as the functions corresponding to the rows of G. Due to orthonormality of $\{f_n\}$ we get

$$\|g_i^k\|^2 = \sum_{j=n}^{\bar{n}} (a_{ij})_k^2.$$

Let $Y_m \subset X$ denote the m-optimal approximating subspace for $\mathcal{F}$ with suitable basis $\{y_i\}_{i=1}^m \subset X$. Let $\bar{Y}_m$ be the restriction of Y to the coordinates $n \dots \bar{n}$, *i.e.*

$$\bar{y}_i := \sum_{j=n}^{\bar{n}} \langle y_i, f_j \rangle f_j, i = 1, \dots m, \quad \bar{Y}_m := \mathrm{span}\{\bar{y}_i\}_{i=1}^m.$$

Set $\bar m := \dim(\bar Y_m) \le m$ and let $\{\phi_i\}_{i=1}^{\bar m}$ be an orthonormal basis of $\bar Y_m$. Then

$$\bar m = \sum_{i=1}^{\bar m} \|\phi_i\|^2 = \sum_{i=1}^{\bar m}\sum_{j=n}^{\bar n} \langle \phi_i, f_j\rangle^2 = \sum_{j=n}^{\bar n}\sum_{i=1}^{\bar m} \langle \phi_i, f_j\rangle^2 .$$

Therefore, there exists a $j^* \in \{n,\dots,\bar n\}$ with

$$\sum_{i=1}^{\bar m} \langle \phi_i, f_{j^*}\rangle^2 \le \frac{\bar m}{\bar n - n + 1} < \frac{m}{n+qm-n} = \frac{1}{q}\cdot \tag{4.3}$$

Set $\bar g_i^k := P_{\bar Y_m} g_i^k$ the orthogonal projection of g_i^k on $\bar Y_m$. We introduce $\bar a_{ij} \in \mathbb{R}^{K+1}$ as the coefficient vectors of $\bar g_i^k$ by

$$(\bar a_{ij})_k := \langle \bar g_i^k, f_j\rangle, \quad k = 0,\dots K,\ i,j = n,\dots,\bar n.$$

Let $j \in \{n,\dots,\bar n\}$, then we obtain with Proposition 3.6 iv), monotonicity of $(\sigma_{T,j})$, and assumption (4.1)

$$\|a_{jj}\|_W^2 \ge \frac{\gamma^2\sigma_{T,j}^2}{K+1} \ge \frac{\gamma^2\sigma_{T,n+qm}^2}{K+1} \ge \frac{\theta^2\gamma^2\sigma_{T,n}^2}{K+1}\cdot \tag{4.4}$$

For j^* we bound the projected coefficients with Cauchy–Schwarz and (4.3):

$$\begin{aligned}(\bar a_{j^*j^*})_k = \langle \bar g_{j^*}^k, f_{j^*}\rangle = \left\langle \sum_{l=1}^{\bar m} \langle g_{j^*}^k, \phi_l\rangle \phi_l, f_{j^*}\right\rangle &= \sum_{l=1}^{\bar m} \langle g_{j^*}^k, \phi_l\rangle \langle \phi_l, f_{j^*}\rangle\\ &\le \left(\sum_{l=1}^{\bar m} \langle g_{j^*}^k, \phi_l\rangle^2\right)^{1/2} \left(\langle \phi_l, f_{j^*}\rangle^2\right)^{1/2} \le \|g_{j^*}^k\| q^{-1/2}.\end{aligned}$$

This allows to bound the coefficient vector norms with the right inequality of Proposition 3.6 v)

$$\begin{aligned}\|\bar a_{j^*j^*}\|_W^2 = \sum_{k=0}^{K} w^k (\bar a_{j^*j^*})_k^2 &\le \sum_{k=0}^{K} w^k \|g_{j^*}^k\|^2 q^{-1} = \sum_{k=0}^{K} w^k \sum_{j=n}^{\bar n} (a_{j^*j})_k^2 q^{-1}\\ &= q^{-1}\sum_{j=n}^{\bar n} \|a_{j^*j}\|_W^2 \le q^{-1}\sum_{j=n}^{\infty} \|a_{j^*j}\|_W^2 \le q^{-1}\sigma_{T,n}^2. \end{aligned}\tag{4.5}$$

With the definition of q it is simple to observe that $2q^{-1/2} \le \gamma\theta/\sqrt{K+1}$. This concludes the proof with (4.4), (4.5) the triangle inequality, orthonormality of f_{j^*}, Cauchy–Schwarz and the best-approximation property of Y_m:

$$\begin{aligned} q^{-1/2}\sigma_{T,n} &= 2q^{-1/2}\sigma_{T,n} - q^{-1/2}\sigma_{T,n} \le \frac{\gamma\theta}{\sqrt{K+1}}\sigma_{T,n} - q^{-1/2}\sigma_{T,n}\\ &\le \|a_{j^*j^*}\|_W - \|\bar a_{j^*j^*}\|_W \le \|a_{j^*j^*} - \bar a_{j^*j^*}\|_W\\ &= \left(\sum_{k=0}^{K} w^k \langle g_{j^*}^k - \bar g_{j^*}^k, f_{j^*}\rangle^2\right)^{1/2} \le \left(\sum_{k=0}^{K} w^k \|g_{j^*}^k - \bar g_{j^*}^k\|^2 \|f_{j^*}\|^2\right)^{1/2}\\ &\le \left(\sum_{k=0}^{K} w^k \|g_{j^*}^k - P_{Y_m} g_{j^*}^k\|^2\right)^{1/2} \le \left(\sum_{k=0}^{K} w^k d_m^2\right)^{1/2} = \sqrt{T} d_m. \end{aligned}$$

□

4.2. Convergence rates

With the previous result, the convergence rate statements of [1] can be adopted. The first statement is that algebraic convergence of the Kolmogorov n-widths implies algebraic convergence of the POD–Greedy approximation error with the same exponent but different multiplicative constant.

Proposition 4.3 (Algebraic convergence of the POD–Greedy)**.**
If $d_n(\mathcal{F}) \leq Mn^{-\alpha}$ for some $\alpha, M > 0$ and all $n \in \mathbb{N}$ and $d_0(\mathcal{F}) \leq M$ then

$$\sigma_{T,n}(\mathcal{F}_T) \leq CMn^{-\alpha}, \quad n > 0 \tag{4.6}$$

with $C := \sqrt{qT}(\rho q)^\alpha$, $q := \lceil 2\gamma^{-1}\theta^{-1}\sqrt{K+1}\rceil^2$ $\rho := \lceil 2(1-\theta^{1/\alpha})^{-1}\rceil$ for arbitrarily chosen $\theta \in (0,1)$ and γ the parameter of the weak POD–Greedy algorithm.

The statement is a slight generalization of the corresponding statement for the Greedy–algorithm in [1], which uses the fixed choice $\theta := 2^{-\alpha}$ implying $\rho = 4$. If θ is chosen, *e.g.* to be the minimizer of C, this multiplicative constant C can be orders of magnitude smaller. In terms of approximation rates, the size of the constant is irrelevant. However, in RB-methods, ultimately a small N is desired possibly with guaranteed error statement. Such rigorous error bounds can be obtained from the error rate statements, as soon as Kolmogorov n-width estimates are available. In this view, a decrease of the constants will be useful, as it reduces such final error bounds. In this respect, our generalization also directly allows a slight improvement of the reference result.

Proof of Propropotion 4.3. We set $q := \lceil 2\gamma^{-1}\theta^{-1}\sqrt{K+1}\rceil^2$ of the form required by Lemma 4.1. We note that for $n = 0$ we have by definition $X_0 := \{0\}$ and $P_{T,0}u = 0, u \in X_T$ hence

$$\sigma_{T,0}(\mathcal{F}_T) = \sup_{u\in\mathcal{F}_T} \|u\|_T = \sup_{u\in\mathcal{F}_T} \sqrt{\sum_{k=0}^K w^k \|u^k\|^2} \leq \sup_{f\in\mathcal{F}} \sqrt{\sum_{k=0}^K w^k \|f\|^2} = \sqrt{T} d_0(\mathcal{F}).$$

With the choice $N_0 := \rho q$ we see that (4.6) holds for all $n \leq N_0$:

$$\sigma_{T,n} \leq \sigma_{T,0} \leq \sqrt{T} d_0 \leq \sqrt{T} M \leq \sqrt{T} M N_0^\alpha n^{-\alpha} = \sqrt{T}(\rho q)^\alpha M n^{-\alpha} \leq CMn^{-\alpha}.$$

Let N be the smallest integer, for which (4.6) does not hold, *i.e.*

$$CMN^{-\alpha} < \sigma_{T,N}. \tag{4.7}$$

This will lead to a contradiction and hence conclude the proposition. Let m be an integer satisfying (proof of existence is postponed)

$$m > 0 \quad \text{and} \quad N - qm > 0, \tag{4.8}$$

$$(N-qm)^{-\alpha} \quad \leq \quad \theta^{-1} N^{-\alpha}, \tag{4.9}$$

$$\sqrt{qT} M m^{-\alpha} \quad \leq \quad CMN^{-\alpha}. \tag{4.10}$$

We define $n := N - qm$ resulting in $n \in \mathbb{N}$ due to (4.8). As $m \geq 1$ and $q \geq 9$ we have $n < N$, thus n satisfies (4.6). Then, we can relate $\sigma_{T,n}$ and $\sigma_{T,N}$ using (4.9) and (4.7)

$$\sigma_{T,n} \leq CMn^{-\alpha} \leq CMN^{-\alpha}\theta^{-1} < \theta^{-1}\sigma_{T,N} = \theta^{-1}\sigma_{T,n+qm}.$$

Then, Lemma 4.1 implies $\sigma_{T,n} \leq \sqrt{qT} d_m$, which in combination with (4.10) results in

$$\sigma_{T,N} \leq \sigma_{T,n} \leq \sqrt{qT} d_m \leq \sqrt{qT} M m^{-\alpha} \leq CMN^{-\alpha}$$

being the desired contradiction to (4.7).

It remains to show the existence of an m satisfying (4.8)–(4.10). For this, we set

$$m := \left\lfloor \frac{N}{q}(1-\theta^{1/\alpha}) \right\rfloor.$$

Concerning (4.8), we immediately note that $m < \frac{N}{q}$ and herewith $N - qm > 0$. For showing $m \geq 1$, we note the following equivalence:

$$m \geq 1 \iff \frac{N}{q}(1-\theta^{1/\alpha}) \geq 1 \iff \left(1 - \frac{q}{N}\right)^{\alpha} \geq \theta. \tag{4.11}$$

By definition of ρ and N_0 we note that

$$2(1-\theta^{1/\alpha})^{-1} \leq \rho \iff \left(1 - \frac{2q}{\rho q}\right)^{\alpha} \geq \theta \implies \left(1 - \frac{q}{N_0}\right)^{\alpha} \geq \theta.$$

As $N > N_0$ this implies (4.11), hence (4.8) is proven.

For showing (4.9), we note that $m \leq \frac{N}{q}(1-\theta^{1/\alpha})$ implies $N - qm \geq N\theta^{1/\alpha}$. Both sides are positive due to (4.8), hence exponentiation with $-\alpha$ gives (4.9).

In order to verify (4.10), we first note that by definition we have $\rho \geq 2(1-\theta^{1/\alpha})$, thus $1-\theta^{1/\alpha} \geq \frac{2}{\rho}$. Further, the definition of N_0 implies $q = \frac{N_0}{\rho} < \frac{N}{\rho}$. These two auxiliary results allow to derive:

$$qm \geq q\left(\frac{N}{q}(1-\theta^{1/\alpha}) - 1\right) = N(1-\theta^{1/\alpha}) - q \geq N\frac{2}{\rho} - \frac{N}{\rho} = \frac{N}{\rho}\cdot$$

Therefore, $(\frac{N}{m})^{\alpha} \leq (\rho q)^{\alpha}$, which gives (4.10):

$$\sqrt{qT} M m^{-\alpha} \leq \sqrt{qT} M \left(\frac{N}{m}\right)^{\alpha} N^{-\alpha} \leq \sqrt{qT} M (\rho q)^{\alpha} N^{-\alpha} \leq CMN^{-\alpha}. \qquad \square$$

The next statement is that exponential convergence of the Kolmogorov n-widths implies exponential convergence of the POD–Greedy error sequence with slightly slower decay and larger multiplicative constant. As the modifications compared to the corresponding statement of [1] only consist of a change of constants, we refrain from the detailed proof in the main text, but refer to the appendix.

Proposition 4.4 ((Sub)-exponential convergence of the POD–Greedy)**.** *If $d_n(\mathcal{F}) \leq M\mathrm{e}^{-an^{\alpha}}$ for $n \geq 0, M, a, \alpha > 0$, then*

$$\sigma_{T,n}(\mathcal{F}_T) \leq CM\mathrm{e}^{-cn^{\beta}}, \quad n \geq 0 \tag{4.12}$$

for $\beta := \frac{\alpha}{\alpha+1}$, arbitrary $\theta \in (0,1)$, $c := \min(|\ln(\theta)|, \frac{a}{(4q)^{\alpha}})$, $C := \max(\mathrm{e}^{cN_0^{\beta}}\sqrt{T}, \sqrt{qT})$, $q := \lceil 2\gamma^{-1}\theta^{-1}\sqrt{K+1}\rceil^2$, $N_0 := \lceil (8q)^{\alpha+1}\rceil$ and γ the constant of the weak POD–Greedy algorithm.

5. Conclusion

In the convergence analysis above, we restricted to the case $l = 1$, *i.e.* only 1 eigenmode is added in each iteration of the POD–Greedy algorithm. In practice, also generalizations are used that include a number of $l > 1$ modes at each iteration. Generalizations of the results could be formulated for these cases by only considering $n \in l\mathbb{N}$ and replacing the subscripts accordingly. For $l = K + 1$ all POD–modes are inserted at once at each POD–Greedy extension step. In this case, the selected trajectory u_n is approximated exactly as $\mathrm{span}\{u_n^k - P_{n-1}u_n^k\}_{k=0}^K = \mathrm{span}\{\varphi_k(u_n - P_{T,n-1}u_n)\}_{k=0}^K$. In this case, the matrix representation of the POD–Greedy algorithm is lower block-triangular.

The proof of the convergence rates of the POD–Greedy algorithm is a step towards theoretical explanation why the method works well in practice, in particular in RB-methods. Herewith it provides a sound foundation for the initially heuristic algorithm. In the original study [1] further properties and variants of the Greedy algorithm are treated, *e.g.* robustness is proven, which takes into account different numerical approximation errors. The same extensions and investigations might be performed for the POD–Greedy algorithm.

An interesting and urging subsequent question is to provide estimates of the Kolmogorov n-width decay rate for certain classes of time-dependent parametric PDEs. Example 3.5 given in this study already illustrates that there exist cases of non-decaying eigenvalue spectrum (transport of discontinuities), but also well behaved examples (stationary processes). The restriction of the algorithm to time-dependent PDEs raises further interesting questions on dependency of the eigenvalues, constants, decay rate, etc. on the choice of the time discretization. This certainly will require a different formal framework, introducing spaces with certain time-regularity rather than only spaces of sequences. Such detailed investigations will be subject to future work.

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A. Proof of exponential convergence rate

Here, we reproduce the proof of the (sub)exponential convergence rate statements from [1] with slight adjustment of constants adopted to our case.

Proof of Propropotion 4.4, (Sub)-Exponential Convergence Rate of POD–Greedy. As in the previous proof, we use $\sigma_{T,0} \le \sqrt{T} d_0$ and $d_0 \le M$ to verify that (4.12) holds for all $n \le N_0$:

$$\sigma_{T,n} \le \sigma_{T,0} \le \sqrt{T} M \mathrm{e}^{cN_0^\beta} \mathrm{e}^{-cN_0^\beta} \le CM\mathrm{e}^{-cn^\beta}.$$

Let $N > N_0$ be the smallest integer, such that (4.12) does not hold, *i.e.*

$$\sigma_{T,N} > CM\mathrm{e}^{-cN^\beta}. \tag{A.1}$$

Let there be an $m \in \mathbb{N}$ (proof of existence is postponed) satisfying

$$\mathrm{e}^{c(N-qm)^\beta} \mathrm{e}^{-cN^\beta} \ge \theta, \tag{A.2}$$

$$N - qm \ge 1, \tag{A.3}$$

$$\sqrt{qT} M \mathrm{e}^{-am^\alpha} \le CM\mathrm{e}^{-cN^\beta}. \tag{A.4}$$

Then, $n := N - qm \in \mathbb{N}$ due to (A.3) and we get with (A.2), (A.1)

$$\sigma_{T,n} \le CM\mathrm{e}^{-cn^\beta} \le CM\theta^{-1}\mathrm{e}^{-cN^\beta} < \theta^{-1}\sigma_{T,N} = \theta^{-1}\sigma_{T,n+qm}.$$

Then we can apply Lemma 4.1 and obtain with (A.4)

$$\sigma_{T,N} \le \sigma_{T,n} \le \sqrt{qT} d_m \le \sqrt{qT} M \mathrm{e}^{-am^\alpha} \le CM\mathrm{e}^{-cN^\beta},$$

which contradicts (A.1).

It remains to show the existence of a suitable m satisfying (A.2)–(A.4). For this we set

$$m := \left\lfloor \frac{N^{1-\beta}}{2q} \right\rfloor.$$

As $\beta \in (0,1)$, we have $m \le N/(2q)$ and obtain (A.3)

$$N - qm \ge N - q\frac{N}{2q} = N/2 \ge 1.$$

Using the mean value theorem, there exists a $\xi \in (N - qm, N)$ such that

$$N^\beta - (N-qm)^\beta = \beta\xi^{\beta-1}qm \leq \beta\left(\frac{N}{2}\right)^{\beta-1}qm \leq \frac{N^{1-\beta}}{2}\beta\left(\frac{N}{2}\right)^{\beta-1} \leq 2^{-\beta}\beta \leq 2^{-\beta}2^\beta = 1.$$

Here we used that $\xi \geq N/2$, $qm \leq N^{1-\beta}/2$ and $\beta \leq 2^\beta$. Then, as $c \leq |\ln\theta|$, we obtain (A.2).

For proving (A.4) we note that $\sqrt{qt} \leq C$ by definition of C, and it remains to show that $am^\alpha \geq cN^\beta$. As $N > N_0$ one can see that $m > 4$ is sufficiently large to imply

$$m = \lfloor\frac{N^{1-\beta}}{2q}\rfloor > \frac{N^{1-\beta}}{4q}\cdot$$

With this we conclude

$$am^\alpha - cN^\beta \geq a\left(\frac{N^{1-\beta}}{4q}\right)^\alpha - cN^\beta = a\frac{N^\beta}{(4q)^\alpha} - cN^\beta = \left(\frac{a}{(4q)^\alpha} - c\right)N^\beta \geq 0,$$

as $c \leq a/(4q)^\alpha$ by definition. □

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