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Karhunen–Loève's truncation error for bivariate functions

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Abstract

Karhunen–Loève decompositions (KLD) or equivalently Proper Orthogonal Decompositions (POD) of bivariate functions are revisited in this work. We investigate the truncation error first for regular functions trying to improve and sharpen bounds found in Griebel and Harbrecht (2014). But, it happens that (KL)-series expansions are in fact more sensitive to the capacity of fields (we are concerned with) to be well represented by a sum of few products of separated variables functions. We consider this issue very important for approximating some interesting field problems defined as solutions of partial differential equations such as the transient heat problem and the Poisson equation. The main tool, to establish approximation bounds in this type of problems, is linear algebra. We show how the singular value decomposition underlying the (KL)-expansion is connected to the spectrum of some Gram matrices and that the derivation of the corresponding truncation error is related to the spectral properties of these Gram matrices which are structured matrices with low displacement ranks. This methodology allows us to show that Karhunen–Loève's truncation error decreases exponentially fast with respect to the cut-off frequency, for some interesting transient temperature fields despite their lack of smoothness.

Keywords: Proper Orthogonal Decompositions; Karhunen–Loève decompositions

1. Introduction

Model Reduction methods developed for data analysis and scientific computing are among the most important enhancing numerical tools in deriving fast and reliable solutions to large scale problems such as, for example, dynamical systems (see [1]). In signal processing for instance, Karhunen–Loève's expansion (KLE) has demonstrated to be a practical procedure for a low dimensional representation of spatiotemporal signals (see [2–4]). This latter particular type of expansion is used in many different fields, although under different names for each scientific community. It is named Proper Orthogonal Decomposition (POD) (see [5]), referred to as Principal Components Analysis (PCA) in statistics and data analysis (see [6–8]) or Singular Value Decomposition (SVD) in linear algebra (see [9]). Although these are the most known terminologies, other denominations do exist. A great amount of work has

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been performed and a wide literature may be found on the application of these techniques to reduce computational cost in several areas which makes them tractable to handle many interesting problems. We refer to the papers, manuscripts and lecture notes in [6,10–16] and references therein. Of course this is not, by far, an exhaustive list of research touching the subject.

Only few papers can be found specifically devoted to the mathematical analysis of the (KL)-truncation error. We reference for instance [17]. The estimate on the truncation error provided in that work is much constrained by the regularity assumptions made on the bivariate field under consideration. The resulting bound establishes that the error is expected to decay faster for smoother fields. This result is no doubt useful, since it concerns a large and well identified class of functions. But the success of an expansion with a small number of terms to produce a good approximation for a given spatiotemporal (bivariate) field has obviously to do with the capacity of that field to be represented by separated time and space functions. This is not necessarily linked to any smoothness property. Proofs of error estimates for general functions seem to be out of reach. However the establishment of sharp estimates for some spatiotemporal fields solutions of some common parabolic or elliptic partial differential systems appears to be more affordable. This is the main target of the present work. For that, the (SVD)-problem underlying the (KL)-expansion is reworded using linear algebra. At least for the type of spatiotemporal functions we are interested in, the advantage is that the underlying eigenvalue problem is initially related to some infinite dimensional structured matrices such as Cauchy or Pick matrices. Their low displacement rank enables us to derive asymptotic expressions for the corresponding eigenvalues, from which we will prove the optimal error estimates.

The guidelines of the paper are as follows. Section 2 recalls the Karhunen–Loève expansion of a given bivariate function, obtained from Mercer's theorem. We point out its most important properties, in particular its optimality in the sense that it is, among all possible expansions, the one that captures the largest fraction of the total energy with a given number of modes. Section 3 revisits the error estimate caused by the truncation of the (KL)-expansion, provided in [17] for regular functions. Then, we illustrate in a simple context how to improve the convergence rate. In Section 4, we investigate the truncation error for the solutions of two transient heat equations. In the first, the temperature field is the one approximated in a transient purely conductive problem without heat source while in the second, the source is defined as a time space separated function. Next, in Section 5 we study the (KL)-approximation of some potentials obtained from the solution of the Poisson equation. In the Appendix, the asymptotic expression of the eigenvalues of some useful Pick matrices are derived.

Notation—Let $X \subset \mathbb{R}^d$ be a given Lipschitz domain. We denote by $L^2(X)$ the space of measurable and square integrable functions on X. The scale of fractional Sobolev spaces $H^\tau(X)$, $\tau > 0$ is defined as in [18].

2. Karhunen–Loève expansion

Assume that $X \subset \mathbb{R}^d$ and $Y \subset \mathbb{R}^s$ are two bounded domains, d and s are integers ≥ 1. Let T be a given function in the Lebesgue space $L^2(X \times Y)$. We are interested in the integral operator with kernel T expressed as

$$\varphi \mapsto B\,\varphi, \qquad (B\,\varphi)(y) = \int_X T(x, y)\varphi(x)\,dx. \tag{1}$$

The operator B maps $L^2(X)$ into $L^2(Y)$, is bounded and has an adjoint operator B^* defined from $L^2(Y)$ into $L^2(X)$ as

$$v \mapsto B^*\,v, \qquad (B^*\,v)(x) = \int_Y T(x, y)v(y)dy. \tag{2}$$

B belongs to the class of Hilbert–Schmidt operators and is thus compact. The self-adjoint operator $A = B^*B$ is also an integral operator whose kernel K is expressed by

$$K(x, \xi) = \int_Y T(x, y)\,T(\xi, y)\,dy.$$

We have $K \in L^2(X \times X)$; A is of course compact. Applying the Hilbert–Schmidt theorem enables the diagonalization of A. There exists a Hilbert basis $(\varphi_m)_{m\geq 0}$ in $L^2(X)$ where φ_m is an eigenvector of A related to a non-negative eigenvalue λ_m, such as

$$A\,\varphi_m = \lambda_m\,\varphi_m, \quad \forall m \geq 0. \tag{3}$$

Assume that the sequence $(\lambda_m)_{m\geq 0}$ is positive, which means that B is injective. We retain this assumption to maintain the focus on the main objectives of the paper and alleviate the exposition as much as possible. When ordered decreasingly, the sequence $(\lambda_m)_{m\geq 0}$ necessarily decays toward zero. A straightforward effect of the diagonalization of the operator A is the following singular value decomposition of the operator B.

Lemma 2.1. *There exists a system* $(\varphi_m, \upsilon_m, \sigma_m)_{m\geq 0}$ *such that* $(\varphi_m)_{m\geq 0}$ *is an orthonormal basis in* $L^2(X)$, $(\upsilon_m)_{m\geq 0}$ *an orthonormal system in* $L^2(Y)$ *and* $(\sigma_m)_{m\geq 0}$ *a sequence of nonnegative real numbers such that*

$$B\,\varphi_m = \sigma_m\,\upsilon_m, \qquad B^*\,\upsilon_m = \sigma_m\,\varphi_m.$$

The sequence $(\sigma_m)_{m\geq 0}$ *is ordered decreasingly and decays toward zero.*

Proof. It is a direct consequence of the spectral decomposition of A. The sequence $(\sigma_m)_{m\geq 0}$ are the singular values of B. In particular, we have $\sigma_m = \sqrt{\lambda_m}$ for all $m \geq 0$. We refer to [19] for a detailed proof. ■

Remark 2.1. The multiplicity of each non vanishing singular value is finite due to the compactness of the operator B.

The positivity of the operator A makes of the kernel K a Mercer kernel. Using Mercer's theorem yields the following decomposition (see [20])

$$K(x,\xi) = \sum_{m\geq 0} \lambda_m \varphi_m(x)\varphi_m(\xi), \quad \forall (x,\xi) \in X \times X.$$

A direct result is the Karhunen–Loève expansion, currently used in the analysis of stochastic processes (see [21,22]). It is more commonly known as the Proper Orthogonal Decomposition in the partial differential equations literature with the related acronym (POD).

Corollary 2.2. *The following expansion holds*

$$T(x,y) = \sum_{m\geq 0} \sigma_m\ \varphi_m(x)\upsilon_m(y), \quad \forall (x,y) \in X \times Y.$$

Remark 2.2. Considering the functions $w_m = \sigma_m \upsilon_m$, the Karhunen–Loève decomposition may be put under the following form

$$T(x,y) = \sum_{m\geq 0} \varphi_m(x) w_m(y), \quad \forall (x,y) \in X \times Y,$$

with the system $(w_m)_{m\geq 0}$ being orthogonal and

$$w_m(y) = \int_X T(x,y)\varphi_m(x)\,dx, \quad \forall y \in Y.$$

The quality of the function T to be accurately represented by a truncated expression of separated variable functions is tightly related to the sequence of singular values $(\sigma_m)_{m\geq 0}$ and in particular to its decreasing rate. We will use in some places the notation

$$T = \sum_{m\geq 0} \varphi_m \otimes w_m.$$

Remark 2.3. The function T_M defined by the truncated sum with a cut-off equal to M is the Karhunen–Loève approximation (*KL-approximation*) of function T. The orthogonality property gives rise to the following estimate

$$\frac{\|T - T_M\|_{L^2(X\times Y)}}{\|T\|_{L^2(X\times Y)}} = \sqrt{\frac{\sum_{m\geq M+1} \lambda_m}{\sum_{m\geq 0} \lambda_m}}. \tag{4}$$

The decaying rate of the eigenvalues $(\lambda_m)_{m\geq 0}$ determines therefore the quality of the truncation.

Remark 2.4. In many areas and in particular in fluid mechanics where model reduction is highly recommended for the determination of the coherent characteristics of turbulent flows for instance, the KL-decomposition is frequently used. When it is applied for the representation of a dynamical field $T = T(x,t)$, the (space-) modes $(\varphi_m)_{m\geq 0}$ are called the coherent structures. They contain spatial features of the dynamical system (*see* [16]).

3. Truncation error

A brief discussion is conducted here about the approximation error. We focus on some particular situations to provide the key-ideas relevant for the estimation of this truncation error. We need beforehand an important result on Karhunen–Loève's approximation.
Let $(\psi_m)_{m\geq 0}$ be a Hilbertian basis in $L^2(X)$. We set

$$u_m(y) = \int_X T(x,y)\psi_m(x)\,dx, \quad \forall y \in Y.$$

Then, we define

$$S_M = \sum_{0\leq m\leq M} \psi_m \otimes u_m.$$

The following estimate holds

$$\|T - T_M\|_{L^2(X\times Y)} \leq \|T - S_M\|_{L^2(X\times Y)}. \tag{5}$$

We refer for instance to [2,3,23] for a detailed proof.

Among all the approximations of the field T by sums similar to the one determining S_M, the KL-approximation is the one that gets the minimum of the L^2-norm of the approximation error. The abstract bound in (5) suggests that there is a connection between the regularity of the function T and the approximation error. This issue has been recently addressed in [17]. We noticed that the result stated there lacks optimality. Below, we expose briefly the way to improve that proof. For that, we start with a simple case to provide clues for such improvement.

Let $I =]-1,1[$ and fix $X = I$. Then, consider $(L_k)_{k\geq 0}$ the Legendre polynomials (see [24]). Actually, we rather work with the normalized polynomials

$$L_m^*(x) = \frac{L_m(x)}{\|L_m\|_{L^2(I)}} = \sqrt{m+\frac{1}{2}}L_m(x), \quad \forall x \in I.$$

The family $(L_m^*)_{m\geq 0}$ is a Hilbert basis in $L^2(I)$. Then, the following expansion holds

$$T(x,y) = \sum_{m\geq 0} L_m^*(x)\tau_m(y), \quad \forall (x,y) \in I\times Y, \tag{6}$$

with the functions $(\tau_k)_{k\geq 0}$ given by

$$\tau_m(y) = \int_I T(x,y)L_m^*(x)\,dx, \quad \forall y \in Y.$$

Recall that T_M stands for the KL-approximation.

Proposition 3.1. *Assume that $T \in H^\tau(I, L^2(Y))$ for some real number $\tau \geq 0$. Then, the following bound holds*

$$\|T - T_M\|_{L^2(I\times Y)} \leq C_T\, M^{-\tau}.$$

Proof. Consider the function

$$S_M(x,y) = \sum_{0\leq k\leq M} L_k^*(x)\tau_k(y), \quad \forall (x,y) \in I\times Y.$$

Recalling for the abstract estimate (5), we have

$$\|T - T_M\|_{L^2(I\times Y)} \le \|T - S_M\|_{L^2(I\times Y)}.$$

Observe that $S_M(\cdot, y)$ is obtained by the orthogonal projection of $T(\cdot, y)$ on the space of polynomial with degree $\le M$. First, let j be an integer. Consider that $T \in H^j(I, L^2(Y))$, then by Fubini theorem we obtain that $\partial_x^{(j)} T \in L^2(I \times Y)$. Owing to [25, Chapter III, Theorem 1.2], we have that

$$\|T(\cdot, y) - S_M(\cdot, y)\|_{L^2(I)} \le C\, M^{-j}\, \|\partial_x^{(j)} T(\cdot, y)\|_{L^2(I)}, \quad \forall y \in Y.$$

Notice that C does not depend on y. Operating the square power and integrating on the variable $y \in Y$ completes the proof for $\tau = j$. As shown in [25, Chapter III], the extension to fractional Sobolev spaces $H^\tau(I, L^2(Y))$, with $\tau \in \mathbb{R}_+$, is achieved by Hilbertian interpolation. ■

Remark 3.1. The convergence rate given in [17] is not the best one could obtain. Particularized to our case, the bound obtained in [17, Theorem 3.4] would be $C_T\, M^{1/2-\tau}$. This is not optimal because of the extra-term $M^{1/2}$. The proof proposed in there is biased because it relies on the estimates of the singular values of the integral operator B. This seems not to be the right way to follow. The proof should be tackled directly, through estimate (5) and using the tensorized argument of [25, Chapter III, Théorème 2.4].

Remark 3.2. The bound obtained in Proposition 3.1 could not be substantially improved for general functions. To support this statement, consider the case $Y = I$ and the function

$$T(x, y) = \sum_{m\ge 2} L_m^*(x)\tau_m(y) = \sum_{m\ge 2} \frac{1}{m^2 \ln m} L_m^*(x) L_m^*(y), \quad \forall (x, y) \in I \times I.$$

It is readily checked that $\partial_x T$ belongs to $L^2(I \times I)$ and $T \in H^\tau(I, L^2(I))$. Moreover, we have that $T \notin H^1(I, L^2(I))$ for $\tau > 1$. The orthogonality of the Legendre polynomial yields that the infinite sum determining T is precisely the Karhunen–Loève expansion. The KL-approximation is thus the truncation

$$T_M(x, y) = \sum_{2\le m\le M} \frac{1}{m^2 \ln m} L_m^*(x) L_m^*(y), \quad \forall (x, y) \in I \times I.$$

Evaluating the approximation error yields the following bound

$$\|T - T_M\|_{L^2(I\times I)} \le C_T\, (M^{3/2} \ln M)^{-1}.$$

This is close to the worst bound predicted by our proposition which is M^{-1}. Proceeding like in [25, Chapter III, Remark 1.4], it would possible to show that Proposition 3.1 cannot be improved.

The bound exhibited in Proposition 3.1 relies fundamentally on the smoothness assumption of the function to approximate. However, for some remarkable functions with only moderate regularity, an effective estimate should account also for the specific contribution of the Karhunen–Loève expansion. For that, we need to look closer to the singular values $(\sigma_m)_{m\ge 0}$ of the operator B or equivalently into the eigenvalues $(\lambda_m)_{m\ge 0}$ of the operator A. It can be checked out that these $(\lambda_m)_{m\ge 0}$ are the eigenvalues of the Gram matrix

$$\mathcal{G} = (g_{km})_{k,m\ge 0} = \big((\tau_k, \tau_m)_{L^2(Y)}\big)_{k,m\ge 0}.$$

Their magnitude is directly dependent on the size of the entries of $\mathcal{G}$. This in turn is related to the smoothness of T. Next, we analyze the influence of the geometry of the family $(\tau_k)_{k\ge 0}$, and in particular of its orthogonality defect. We expose our study for two important classes of bivariate functions that arise as solutions of widely spread parabolic and elliptic boundary value problems (see [26]).

Remark 3.3. Regarding this specific orthogonality point, if the functions $(\tau_k)_{k\ge 0}$ are orthogonal then the Gram matrix $\mathcal{G}$ is diagonal and according to Remark 3.2, the sum (6) is nothing else than the Karhunen–Loève expansion. Thus the result of Proposition 3.1 cannot be improved.

4. Transient temperature

We investigate two examples of transient heat transfer problems. Writing down the temperature field as a Fourier series is as old as the first closed expressions of the solutions of the heat equation. The infinite Fourier sum involves separation of both time and space variables. Starting from this Fourier series expression, our aim is to come up with a new infinite sum representation that enhances that separation of time and space variables so that a low truncation is possible, preserving the main features of the temperature field with high accuracy. The purpose is therefore to illustrate the impact of the orthogonality defect suffered by the Fourier expansion of the field T and to show how the Karhunen–Loève decomposition allows a better expression regarding the accuracy of variables separation.

4.1. Heat equation with no source term

Assume that $J =]0, b[$ and Ω, a regular domain in $\mathbb{R}^s$, are the variation intervals of the independent variables t the time variable and x the spatial variable. In this example, no source is present. The problem of interest is then defined as: *find a temperature field T such that*

$$\begin{aligned}
&\partial_t T - \text{div}\,(\gamma \nabla T) + \beta T = 0, \quad \text{in } \Omega \times J,\\
&T = 0, \quad \text{in } \partial\Omega \times J,\\
&T(\cdot, 0) = a(\cdot), \quad \text{in } \Omega,
\end{aligned}$$

where γ the conduction parameter and β is the heat transfer coefficient are both space varying and positive. The temperature field, solution of this problem can be expressed using Fourier series. Consider thus the eigenvalue problem:

$$\begin{aligned}
&-\text{div}\,(\gamma \nabla e) + \beta e = re, \quad \text{in } \Omega,\\
&e = 0, \quad \text{on } \partial\Omega.
\end{aligned} \tag{7}$$

The sequence of eigenvalues $(r_m)_{m\geq 1}$ is positive and grows to infinity like $Cm^{2/s}$ (see [27]). The eigenfunctions $(e_m)_{m\geq 1}$ form an orthonormal basis in $L^2(\Omega)$; it is orthogonal and dense in $H_0^1(\Omega)$ (see [28]). Using this basis, the solution of the boundary value heat problem may thus be written as

$$T(x, t) = \sum_{m\geq 1} a_m e^{-r_m t} e_m(x), \quad \forall (x, t) \in \Omega \times J. \tag{8}$$

Fourier coefficients $(a_m)_{m\geq 1}$ are square summable ($\in \ell^2(\mathbb{R})$). It is easily seen that

$$\|\nabla T\|^2_{L^2(\Omega\times J)} = \frac{1}{2} \sum_{m\geq 1} (a_m)^2 (1 - e^{-2r_m b}) < \infty.$$

There is clearly no more smoothness on T with respect to x unless the decaying rate of the sequence $(a_m)_{m\geq 1}$ is high. The dependence on t is even less regular. Hence, Proposition 3.1 predicts the following bound on the (KL)-approximation error

$$\|T - T_M\|_{L^2(\Omega\times J)} \leq C_a\, M^{-1}.$$

This is far from being satisfactory. Anyway, it is not in accordance with the observations made in many papers (see, e.g., [26]). In fact, the geometry of the system $(e^{-r_m t})_{m\geq 1}$ plays an important role in enhancing the estimate.

Remark 4.1. Before stepping forth, and seeking simplification, we assume that the sequence of eigenvalues $(r_m)_{m\geq 1}$ is increasing. This means that each eigenvalue r_m of the Laplace operator is simple. This is always true in one dimension. In two and three dimensions it often occurs that some of the eigenvalues have a multiplicity higher than one. Handling multiple eigenvalues requires that some slight adaptation be added to the subsequent discussion and does not arise any particular problem.

The system $(e^{-r_m t})_{m\geq 1}$ suffers from a big lack of orthogonality. In fact, it is almost linearly dependent (see [29]). Next, we shall develop some analytical computations to improve that approximation result by taking advantage of the singular value decomposition. We start with the calculation of the kernel K related to A. It is given by

$$K(x,\xi) = \sum_{k\geq 1}\sum_{m\geq 1} a_m a_k \left(\int_{(0,b)} e^{-(r_m+r_k)t}\, dt\right) e_k(x)e_m(\xi)$$
$$= \sum_{k\geq 1}\sum_{m\geq 1} a_k \frac{1-e^{-(r_m+r_k)b}}{r_m+r_k} a_m\, e_k(x)e_m(\xi).$$

Now, we expand the function φ as follows

$$\varphi(x) = \sum_{m\geq 1} f_m e_m(x), \quad \forall x \in \Omega.$$

After replacing in the eigenvalue equation (3), we get

$$\sum_{k\geq 1}\left(\sum_{m\geq 1} a_k \frac{1-e^{-(r_m+r_k)b}}{r_m+r_k} a_m f_m\right) e_k(x) = \lambda \sum_{k\geq 1} f_k\, e_k(x).$$

This eigenvalue problem can be written under a matrix form, as follows

$$\mathcal{G}\boldsymbol{\varphi} = \lambda\boldsymbol{\varphi}. \tag{9}$$

The Gram matrix is defined as $\mathcal{G} = \mathcal{A}\mathcal{C}_b\mathcal{A}$. The entries of different matrices for all $k, m \geq 1$ are provided by

$$c_{km} = \frac{1-e^{-(r_m+r_k)b}}{r_m+r_k}, \qquad a_{km} = a_k\delta_{km}, \qquad g_{km} = a_k c_{km} a_m.$$

The coefficients of the vector $\boldsymbol{\varphi}$ are $(f_m)_{m\geq 1}$. The matrix $\mathcal{C}_b$ is symmetric and positive definite. Finally, the matrix $\mathcal{G}$ is non-negative definite. The kernel $N(\mathcal{G})$ coincides with the kernel $N(\mathcal{A})$. The eigenvalues of such a matrix decay fast toward zero. We refer to [30] and postpone a detailed study of this matrix. We provide here the final result.

Proposition 4.1. *Assume that $a_m = 0, \forall m \geq M$ for a large integer M. The following bound holds*

$$\sigma_m \leq C\|a\|_{L^2(\Omega)} \exp\left(-\frac{\mu m}{\log(r_M)}\right), \quad 1 \leq m \leq M.$$

μ is a positive real number.

Proof. It is provided in the Appendix. ■

Remark 4.2. To have an initial idea about the spectral features of the Gram matrix, we investigate the one dimensional case where $\Omega = (0,\pi)$, $J = (0,\infty)$ and the parameters are $\gamma = 1$ and $\beta = 0$. Thus we derive that $r_m = m^2$. The matrix $\mathcal{C}_\infty$ is of Cauchy type and so are all its principal sub-matrices. Their determinants can hence be calculated explicitly. According to [31], the principal sub-determinant with (large) order M_∞ of $\mathcal{C}_\infty$ is given by

$$\det_{M_\infty} = \frac{\prod_{2\leq k\leq M_\infty}\prod_{1\leq m\leq k-1}(k^2-m^2)^2}{\prod_{1\leq k\leq M_\infty}\prod_{1\leq m\leq M}(k^2+m^2)}.$$

This determinant decays very fast toward zero for growing M_∞. This is an indication of the fast decrease of that the eigenvalues of $\mathcal{C}_\infty$ toward zero.

4.2. Influence of a separated source term

We consider now the case of having a heat source term with a particular structure represented by a separated function on t and x so that $S(x,t) = a(x) \otimes \theta(t)$. In this case, we expect that the temperature field might be represented by a sum of separated functions. This assumption, although true, is not easy to prove The heat model to handle is the following: *find a temperature field T satisfying*

$$\partial_t T - \text{div}\,(\gamma \nabla T) + \beta T = S, \quad \text{in } \Omega \times J,$$
$$T = 0, \quad \text{in } \partial\Omega \times J,$$
$$T(\cdot, 0) = 0, \quad \text{in } \Omega.$$

After some Fourier calculations we come up with the following

$$T(x,t) = \sum_{m\geq 1} a_m \left(\int_J \theta(s) e^{-r_m(t-s)}\, ds \right) e_m(x), \quad \forall (x,t) \in \Omega \times J.$$

Straightforward integral computations yield the following expression for the Mercer kernel K,

$$\begin{aligned} K(x,\xi) &= \int_{(0,b)} T(x,t) T(\xi,t)\, dt \\ &= \sum_{k\geq 1}\sum_{m\geq 1} \frac{a_k a_m}{r_m + r_k} \left(\int_J \int_J \theta(s)\theta(\tau)(e^{-r_m|s\wedge\tau - s|} e^{-r_k|s\wedge\tau-\tau|})\, ds d\tau \right) e_k(x) e_m(\xi) \\ &\quad + \sum_{k\geq 1}\sum_{m\geq 1} \frac{a_k a_m}{r_m + r_k} \left(\int_J \theta(s) e^{-r_k(b-s)}\, ds \right) \left(\int_J \theta(\tau) e^{-r_m(b-\tau)}\, d\tau \right) e_k(x) e_m(\xi). \end{aligned}$$

The notation $s \wedge \tau$ is used for $\max(s,\tau)$. Taking profit from the symmetry of this kernel we may bring it out to a more convenient form

$$\begin{aligned} K(x,\xi) &= \frac{1}{2} \sum_{k\geq 1}\sum_{m\geq 1} \frac{a_k a_m}{r_m + r_k} \left(\int_J \int_J \theta(s)\theta(\tau)(e^{-r_m|\tau - s|} + e^{-r_k|s-\tau|})\, ds d\tau \right) e_k(x) e_m(\xi) \\ &\quad + \sum_{k\geq 1}\sum_{m\geq 1} \frac{a_k a_m}{r_m + r_k} \left(\int_J \theta(s) e^{-r_k(b-s)}\, ds \right) \left(\int_J \theta(\tau) e^{-r_m(b-\tau)}\, d\tau \right) e_k(x) e_m(\xi) \\ &= \sum_{k\geq 1}\sum_{m\geq 1} g_{km} e_k(x) e_m(\xi). \end{aligned}$$

Once the Mercer kernel is explicit, the next point is the determination of the eigenvalues of the operator A. Based on the arguments developed in the previous example, we can rearrange the eigenvalue problem (3) under an algebraic form similar to (9). We need thus to cope with the asymptotics of the eigenvalues of the new Gram matrix $\mathcal{G} = (g_{km})_{k,m\geq 1}$. This can be achieved as in the Appendix. It can be checked that $\mathcal{G}$ satisfies the Lyapunov equation with the same Cauchy-like displacement operator that is

$$\mathcal{R}\mathcal{G} + \mathcal{G}\mathcal{R} = \alpha\eta^T + \eta\alpha^T + \delta\delta^T. \tag{10}$$

The entries of vectors e and d are given by

$$\alpha_m = a_m, \qquad \eta_m = \frac{a_m}{2} \int_J \int_J \theta(s)\theta(\tau) e^{-r_m|\tau-s|}\, ds d\tau \qquad \delta_m = a_m \int_J \theta(s) e^{-r_m(b-s)}\, ds.$$

The displacement rank of Eq. (10) is three. Reproducing the proof in the Appendix yields the following result

Proposition 4.2. *Assume that $a_m = 0, \forall m \geq M$ for a large integer M. The following estimate on the singular values of B holds*

$$\sigma_m \leq C \|a\|_{L^2(\Omega)} \|\theta\|_{L^2(J)} \exp\left(-\frac{\mu m}{\log(r_M)} \right), \quad 1 \leq m \leq M.$$

Remark 4.3. Results by Proposition 4.2 predict that the singular values of the integral operator B decreases rapidly toward zero. The log term in the bound may slow down the decaying rate of convergence. The decreasing rate of $(\sigma_m)_{m\geq 1}$ is however almost exponential at least for the fraction of indices m larger than $\log(M)$. Anyhow, our feeling is that it should be possible to get rid of that log-term, although we were not able of getting the proof.

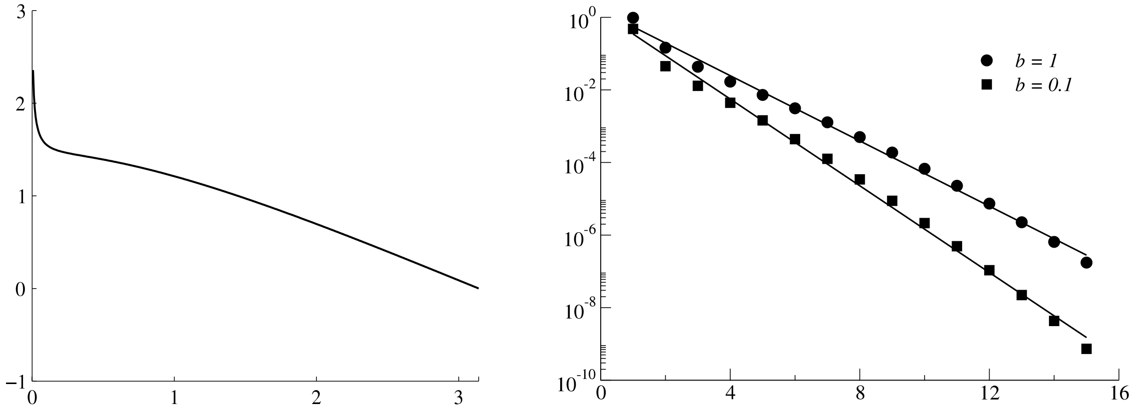

Fig. 1. The initial temperature a (left). Singular values for $b = 1$, $b = 0.1$ (right).

4.3. Numerics

To support the above theoretical findings on the singular values $(\sigma_m)_{m\geq 1}$ of the operator B as the square roots of the eigenvalues of the Gram matrix in the first example, we provide numerical results obtained within MATLAB. We fix $\gamma = 1$ and $\beta = 0$. Then, we have $r_m = m^2$, fix $a_m = 0$, $\forall m > M_\infty$ and

$$a_m = \frac{1}{\sqrt{m}\ln(m+1)}, \qquad m \leq M_\infty.$$

The corresponding function a is depicted in the left panel in Fig. 1. It is in $L^2(I)$ and does not belong to any Sobolev space $H^\tau(I)$ for $\tau > 0$. The slope of the representative curve of $a(\cdot)$ at the vicinity of $x = 0$ suggests that it contains a singularity there.
The non-vanishing part of the Gram matrix $\mathcal{G}$ is thus the principal block of dimension M_∞,

$$g_{km} = \frac{1}{\sqrt{k}\ln(k+1)} \frac{1 - e^{-(k^2+m^2)b}}{k^2 + m^2} \frac{1}{\sqrt{m}\ln(m+1)}, \qquad 1 \leq k, m \leq M_\infty.$$

All the other entries are zeros. Apart from the first M_∞ eigenvalues $(\lambda_m)_{1\leq m\leq M_\infty}$, the others are zero. We compute the singular values $(\sigma_m = \sqrt{\lambda_m})_{1\leq m\leq M_\infty}$ for $M_\infty = 23$. They are represented in Fig. 1, in a semi-logarithmic scale and with different final times $b = 1, 0.1$. The trend observed here seems in accordance with the analysis prediction. The singular values sequence decreases toward zero fast. The shape of the first portion of the curve suggests an exponential decaying.

In the next examples, the space and time intervals are fixed to $I = (0, 1)$ and $J = (0, 1)$. We carry out two simulations where separated source terms are present in the heat equation. They are given by

$$S_1(t, x) = (\theta \otimes a)(x, t) = e^t(x - 0.4),$$
$$S_2(t, x) = (\theta \otimes a)(x, t) = e^t|x - 0.4|.$$

The corresponding solutions are denoted by T_1 and T_2, respectively. The heat problem is discretized by an Euler scheme/Gauss–Lobatto–Legendre spectral method see [25] (the time step is $\delta t = 10^{-2}$ and the polynomial degree is $N = 64$). Then, quadrature formulas are used to evaluate the matrix representation of the operators B and A. Let us emphasize on the fact that in the first source term, separated functions $\theta(\cdot)$ and $a(\cdot)$ are indefinitely smooth. For the second source, $a(\cdot)$ enjoys moderate spacial regularity, since $a \in H^\tau(I)$ with τ no bigger than $3/2$. Our aim is to show that the regularity has not much importance in the separation aptitude of both temperature fields T_1 and T_2. Although their smoothness degrees are deeply different they show the same capacity to separated representation.

To support these claims, we construct the Gram matrix associated with the integral operator A and compute the eigenvalues ([1]). The related singular values are depicted in Fig. 2 in a semi-logarithmic scale. The decreasing rate

[1] The procedure `dsyevd` from LAPACK is called.

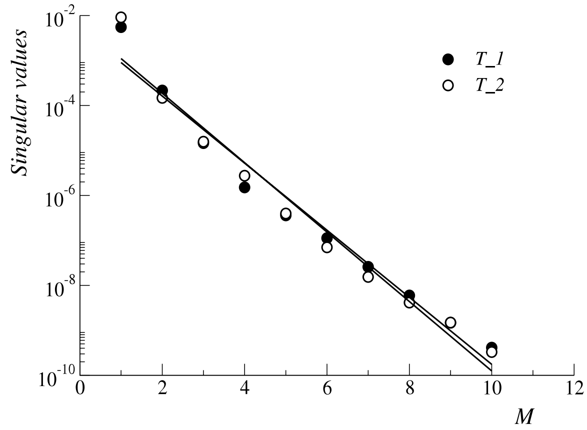

Fig. 2. Singular values for T_1 and T_2.

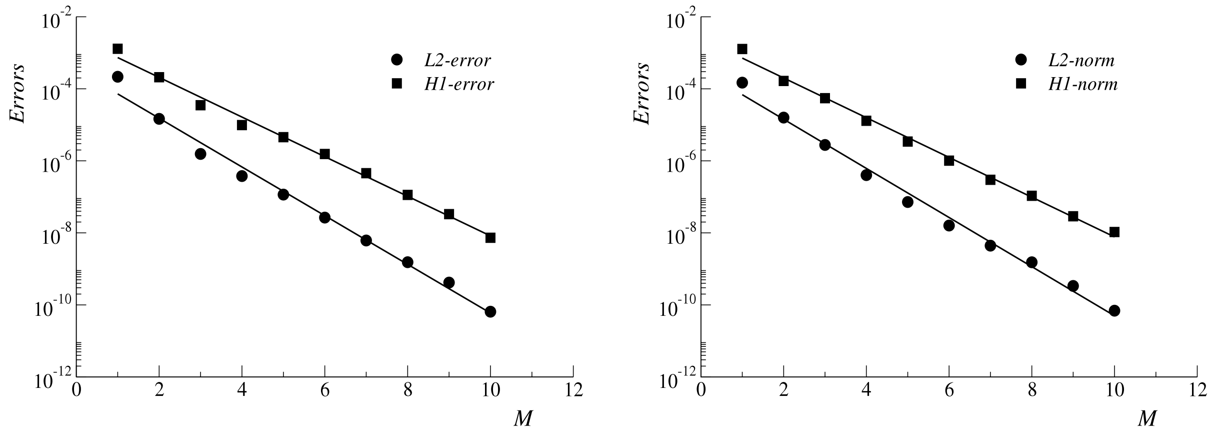

Fig. 3. Truncation errors versus the cut-off M, for T_1 and T_2.

seems to be exponential in both cases as predicted by the analytical study. With these regards, the L^2-errors caused by truncation of the (KL)-expansions are expected to decrease exponentially too. This is confirmed in the error curves depicted in Fig. 3. To figure out the H^1-norm behavior of those truncation errors, we plotted also the H^1-norm of those truncation errors. They decrease exponentially fast too. Notice that so-far no theoretical proofs are available for such result.

In the last example, the source term 'suffers' from a strong coupling between t and x. It is defined as

$$S_3(t, x) = \sqrt{|x - t - 0.3|}.$$

According to the smoothness analysis in [32], the solution of the corresponding heat problem is such that ([2])

$$T_3 \in H^{(3)_-}(I; L^2(J)) \cap L^2(I; H^{(3/2)_-}(J)).$$

The temperature field T_3, solution of the heat equation, is not accessible. As a representation of it, we use a reference computed field. It is obtained by a second order implicit Euler/Legendre spectral discretization of the heat equation. The time step is fixed to $\delta t = 10^{-3}$ and the cut-off frequency for the spectral approximation is fixed to $N = 256$. We guess that the temperature T_3 will show a weaker ability to be represented by a sum of separated functions than the previous temperature fields. The singular values of the operator B are not expected to decay fast, at least not exponentially. They are plotted in Fig. 4 in a *full logarithmic scale*. The decaying rate seems in fact to be polynomial. The polynomial regression tells us that $(\sigma_m)_m$ decreases like $m^{-3.94}$.

[2] The notation $(3)_-$ is used to indicate that the result holds for all Sobolev exponents < 3. The same convention is adopted for $(3/2)_-$.

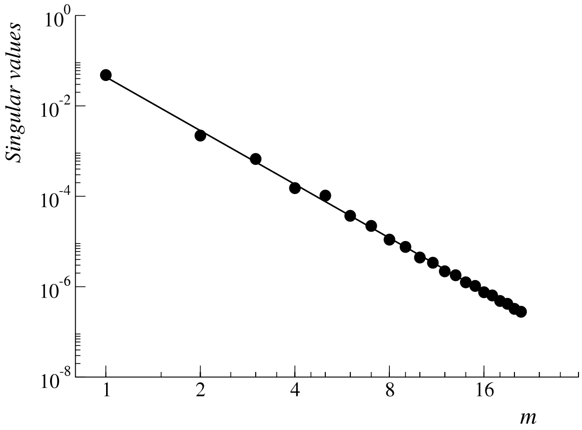

Fig. 4. Singular values for T_3.

According to the estimate (4), the L^2-norm of the truncation error is expected to behave – for lower cut-off frequencies – as

$$\|T - T_M\|_{L^2(I\times J)} \le C\sqrt{\sum_{m\ge M+1}(\sigma_m)^2} \approx C\sqrt{\sum_{m\ge M+1} m^{-7.88}} \approx CM^{-3.44}.$$

The convergence rate of the L^2-error obtained as the slope of the linear regression in the left diagram in Fig. 5 equals $M^{-3.16}$. Theoretical and evaluated rates are slightly close. Furthermore, the H^1-truncation error is provided in the same diagram. The related convergence rate is close to $M^{-2.17}$. Before closing, the target of the error curves in the right panel of Fig. 5 is to conduct a comparison between the Karhunen–Loève approximation of T_3 and the 'space-polynomial' approximation obtained, at each time level $t^n = n(\delta t)$, by the orthogonal projection on $\mathbb{P}_M(I)$, the space of polynomials with degree $\le M$. Both approximations show the same trend. Their convergence rates are close. Indeed, the regressions of these curves yield the rates (3.16, 2.17) for the (L^2, H^1)-error for the Karhunen–Loève approximation and (3.62, 2.56) for the polynomial approximation. As expected in (5), the latter is less accurate than the former.

5. Potentials from Poisson's equation

We investigate here the case of some particular potentials considered in [26, Chapter II]. We denote once again $I =]0, \pi[$ and we set $X = Y = I$. The aim is to study the accuracy of the KL-approximation of the potential

$$V(x, y) = \sum_{k\ge 1}\sum_{m\ge 1}\frac{f_{km}}{k^2+m^2}\sin(kx)\sin(my), \quad \forall (x, y) \in I\times I. \tag{11}$$

The doubly indexed sequence of reals $(f_{km})_{k,m\ge 1}$ is assumed square summable. It may be accounted for as the Fourier coefficients of a function $f \in L^2(I\times I)$. The potential $V \in H^1(I\times I)$ is solution of the Poisson equation set in the square $I\times I$ with homogeneous Dirichlet condition and the function f being the source input: *find a potential field V such that*

$$-\Delta V = f \quad \text{in } I\times I,$$
$$V = 0 \quad \text{in } \partial(I\times I).$$

Analytical computations were carried out again to find the kernel K related to the operator A. Recall that $A = B^*B$ and the kernel of the integral operator B is V. Using (11), and all calculations achieved, the expression we obtain is

$$K(x, \xi) = \sum_{k\ge 1}\sum_{\ell\ge 1}\left(\sum_{m\ge 1}\frac{f_{km}f_{\ell m}}{(k^2+m^2)(\ell^2+m^2)}\right)\sin(kx)\sin(\ell\xi).$$

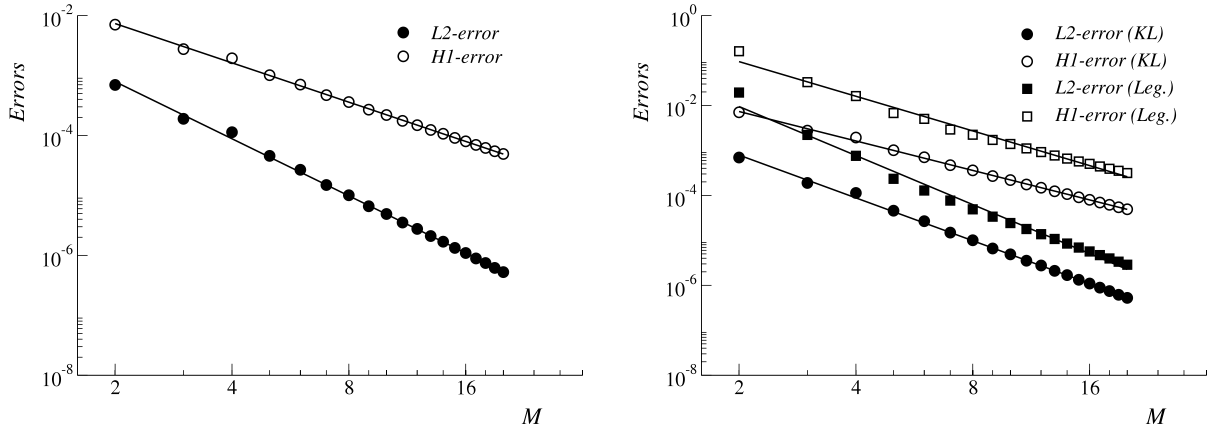

Fig. 5. Karhunen–Loève errors for T_3 (left). Both K.-L. and Legendre polynomial errors (right).

Following the same methodology as above, the eigenvalue equation (3) may be translated into an algebraic form

$$\mathcal{G}\boldsymbol{\varphi} = (\mathcal{F} \circ \mathcal{C})(\mathcal{F} \circ \mathcal{C})^T \boldsymbol{\varphi} = \lambda \boldsymbol{\varphi}.$$

$\mathcal{F}$ is the matrix $(f_{km})_{k,m \geq 1}$ while the entries of $\mathcal{C}$ and $\mathcal{G}$ are given by: for all $k, m, \ell \geq 1$,

$$c_{km} = \frac{1}{k^2 + m^2}, \qquad g_{k\ell} = \sum_{m \geq 1} (f_{km} c_{km})(f_{\ell m} c_{\ell m}).$$

The matrix $\mathcal{C}$ is a Cauchy matrix, symmetric and positive definite. The symbol $\circ$ is for the Hadamard term-to-term product of matrices. Now, assume the function $f = 1$, then $f_{km} = a_k a_m$ with $a_k = \frac{1-(-1)^k}{k}$. The only non vanishing modes are the odd indexed ones. This is because $a_{2k} = 0$ and $a_{2k+1} = \frac{2}{2k+1}$. Thus, we retain only the odd indexes for k and m. However, to alleviate the presentation and with abuse of notations we still write k and m instead of $2k + 1$ or $2m + 1$. As a result, the Hadamard product $\mathcal{F} \circ \mathcal{C}$ may be expressed under a standard product as follows

$$\mathcal{F} \circ \mathcal{C} = \mathcal{A}\mathcal{C}\mathcal{A}$$

with $\mathcal{A} = \text{Diag } (a_k)_{k \geq 1}$. As it is symmetric positive definite its eigenvalues and singular values coincide. The study detailed in the Appendix extends as well here and the sequence of singular values $(\sigma_m)_{m \geq 1}$ decreases exponentially fast. We stress on the fact that the potential V has a moderate Sobolev regularity because of the corner singularities (see [33]). Indeed, $V \in H^\tau(I \times I)$ only for $\tau < 3$. Based on this smoothness, Proposition 3.1 fails to predict the exact behavior of the Karhunen–Loève approximation of the field V. This analysis is readily extended to any data function $f = g \otimes h$ (i.e. $f(x, y) = g(x)h(y)$) or to any linear combination of such kind of functions.

To check out these findings we conduct some simulations using variational spectral method with a Gauss–Lobatto grid containing 65×65 nodes. The singular values and the truncation errors are provided in Fig. 6. A semi-logarithmic scale is adopted. The decaying rate so as the convergence rates of the errors seem to be at least exponential.

To investigate a less favorable example, we turn now to the study of the KL-approximation of the potential V when the data f is a Dirac distribution supported by the first bisector (the line $x - y = 0$). The source f is then defined as $f(x, y) = \delta_{(y-x)}$. Of course, it belongs to $H^{-1}(I \times I)$ without being in $L^2(I \times I)$. Calculating Fourier's expansion of f is straightforward. We obtain that

$$f(x, y) = \delta_{(y-x)} = \frac{2}{\pi} \sum_{m \geq 1} \sin(mx) \sin(my).$$

Inserting Fourier coefficients of f in the expression of the potential V, there comes out that

$$V(x, y) = \frac{1}{\pi} \sum_{m \geq 1} \frac{1}{m^2} \sin(mx) \sin(my), \quad \forall (x, y) \in I \times I. \tag{12}$$

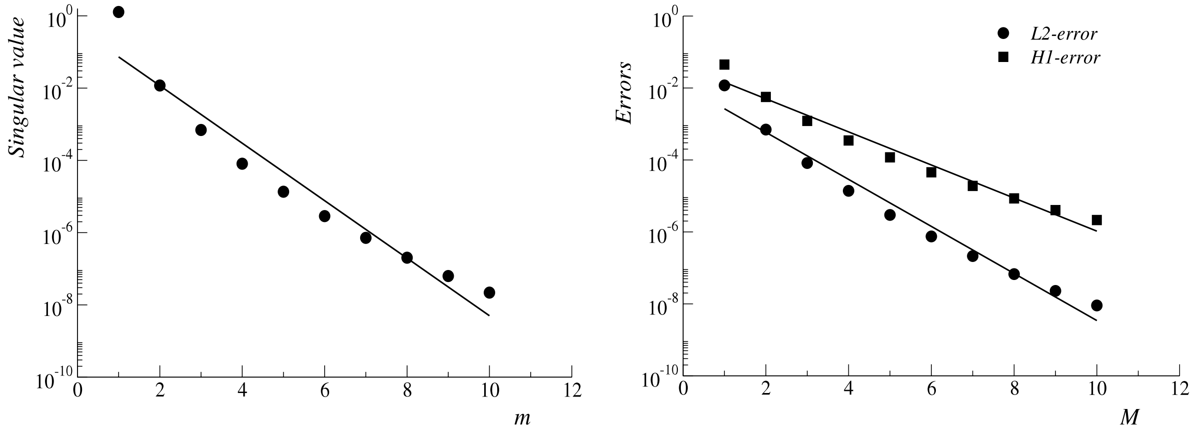

Fig. 6. Singular values for V (left). Truncation errors (right).

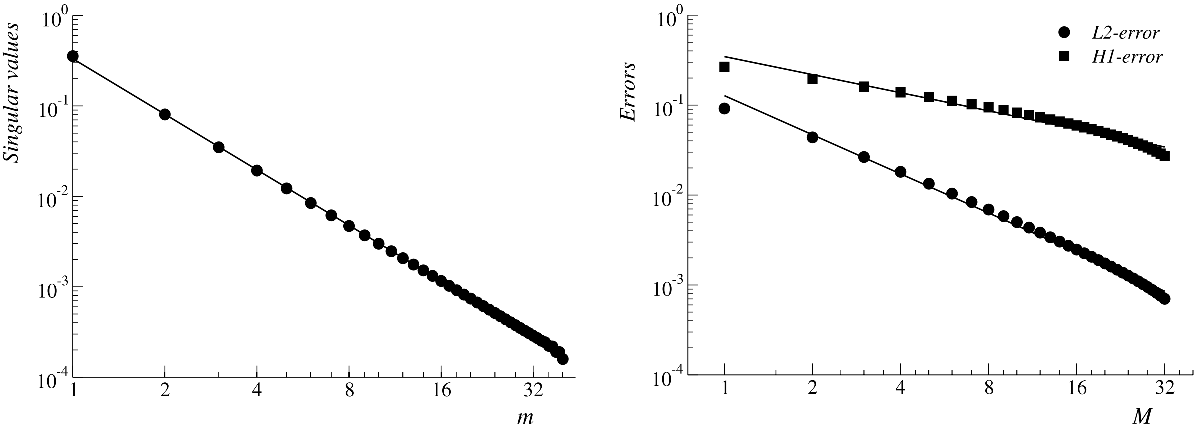

Fig. 7. Singular values for V (left). Truncation errors (right).

This new potential V has a lower regularity than the first. Indeed, we have that $V \in H^\tau(I \times I)$ for $\tau < 3/2$. Now, a closer look at the expansion (12) shows that, due to the orthogonality, the sum is exactly the Karhunen–Loève decomposition of V. Therefore, the KL-approximation error turns out to be the truncation error. We derive easily that

$$M\|V - V_M\|_{L^2(I\times I)} + \|V - V_M\|_{H^1(I\times I)} \le CM^{-1/2}.$$

The properties of the current potential seem to be in the opposite case to the former. The capacity of separating variables t and x is highly reduced.

For users who are interested on the singular values of B, let us observe first that the matrix $\mathcal{F}$ is proportional to the identity that is $\mathcal{F} = \frac{\pi}{2}\mathcal{I}$. The Hadamard product reduces therefore to

$$(\mathcal{F} \circ \mathcal{C}) = \frac{\pi}{4}\text{Diag}\left(\frac{1}{m^2}\right)_{m\ge 1}.$$

The sequence of the singular values $(\sigma_m)_{m\ge 1}$ coincides with the diagonal coefficients and decreases slowly toward zero.

We aim at finding out whether the facts described above are observed when the potential field V is replaced by the approximated solution of the Poisson equation. We use a variational Legendre spectral method to achieve the discretization. The Gauss–Lobatto grid we choose to compute the discrete solution is composed of 65 points per direction. Fig. 7 depict the behavior of the singular values and the truncation errors. The full-logarithmic scale is used for both diagrams. The decreasing rate for the singular values is evaluated to 2.04. The convergence rates of the truncation error are equal to 1.54 and 0.77 for the L^2- and H^1-norms respectively. This is almost in perfect accordance with the predictions.

6. Conclusion

A convergence analysis of the Karhunen–Loève expansion of bivariate functions is developed. We give analytical bounds of the truncation errors for two types of fields. The first corresponds to solutions of transient heat equations and the second is associated with potentials fulfilling the Poisson boundary value problem. The results shown are in accordance with the numerical trends observed in many works. The truncation error decreases exponentially fast with respect to the number of (KL)-modes retained.

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Appendix. Eigenvalues of some Pick matrices

We pursue the asymptotics of the eigenvalues of the Gram matrix $\mathcal{G} = (g_{km})_{k,m\geq 1}$, numerically investigated in Section 3. The entries of $\mathcal{G}$ are re-transcribed as follows

$$g_{km} = a_k \frac{1 - e^{-(r_k+r_m)b}}{r_k + r_m} a_m, \quad \forall k, m \geq 1.$$

Recall that the sequence $(r_k)_{k\geq 1}$ is positive and grows to infinity. The infinite matrix $\mathcal{G}$ is symmetric, compact and positive. Its eigenvalues are expected to decrease toward zero. Having a look for instance to its columns shows that the high indexed ones are almost collinear. This is an indication on a fast decaying of the eigenvalues. To prove such a claim we exploit the fact that $\mathcal{G}$ is a structured matrix in the class of Pick matrices. Denote the diagonal matrix $\mathcal{R} = \text{diag}\,\{r_k\}_{k\geq 1}$ and vectors $\alpha = (a_k)_{k\geq 1}$ and $\alpha' = (a_k e^{-r_k b})_{k\geq 1}$. It is readily checked that the matrix $\mathcal{G}$ satisfies the Lyapunov equation

$$\mathcal{R}\mathcal{G} + \mathcal{G}\mathcal{R} = \alpha\alpha^T - (\alpha')(\alpha')^T. \tag{13}$$

This equation is related to the notion of displacement operators (see [34]). In fact, $\mathcal{G} \mapsto \mathcal{R}\mathcal{G}+\mathcal{G}\mathcal{R}$ is called Cauchy-like displacement operator in the specialized literature. The rank of the matrix $\alpha\alpha^T - (\alpha')(\alpha')^T$ is called the displacement rank of Eq. (13). It equals two.

To work with finite matrices we assume that the sequence (a_m) vanishes after a large rank M, i.e. $a_m = 0, \forall m > M$. All vectors and matrices are therefore truncated in an obvious way The asymptotic expansion of the eigenvalues of $\mathcal{G}$ is strongly connected to the properties of the displacement operator and by then on the diagonal matrix $\mathcal{R}$ and to the displacement rank of (13). Bounds will be derived after applying results that have been reviewed in [35]. The following result holds.

Proposition A.1. *We have that*

$$\sigma_1 \leq C\|\alpha\|_{\ell^2(\mathbb{R})}. \tag{14}$$

The constant C is independent of M.

Proof. Let us first bound the Frobenius norm of $\mathcal{G}$. We have that

$$\|\mathcal{G}\|_F^2 = \sum_{1\leq k,m\leq M} \frac{(a_k)^2(a_m)^2}{(r_k+r_m)^2} \leq \sum_{1\leq k,m\leq M} \frac{(a_k)^2(a_m)^2}{4r_k r_m} = \frac{1}{4}\left(\sum_{1\leq k\leq M} \frac{(a_k)^2}{r_k}\right)^2.$$

Given that $(r_k)_{k\geq 1}$ grows to infinity it comes out that

$$\|\mathcal{G}\|_F \leq C\|\alpha\|^2_{\ell^2(\mathbb{R})}.$$

The bound on the largest eigenvalue $\lambda_1 = (\sigma_1)^2$ of $\mathcal{G}$ is directly obtained

$$\lambda_1 \leq \|\mathcal{G}\|_F \leq C\|\alpha\|^2_{\ell^2(\mathbb{R})}. \tag{15}$$

The bound (14) is established after switching to the square roots. ■

Proposition A.2. *Assume M be large enough. The following bound holds*

$$\sigma_{2i} \leq C\|\alpha\|_{\ell^2(\mathbb{R})} \exp\left(-\frac{\pi^2 i}{2\log(r_M)}\right), \quad 1 \leq i \leq [(M-1)/2].$$

Proof. Let us observe first that the displacement rank of the Lyapunov equation (13) is two. Recalling Theorem 2.1.1 of [35, pp. 39–40] we get the following bound

$$\frac{\lambda_{2i}}{\lambda_1} \leq C \exp\left(-\frac{\pi^2 i}{\log(4\kappa(\mathcal{R}))}\right). \tag{16}$$

The constant C is independent of N. The symbol $\kappa(\mathcal{R})$ is for the condition number of the matrix $\mathcal{R}$. Given that $\kappa(\mathcal{R})$ is easily computed for diagonal matrices, it coincides with the ratio of the maximal and the minimal diagonal terms (r_M/r_1). Hence we obtain that

$$\lambda_{2i} \leq C\lambda_1 \exp\left(-\frac{\pi^2 i}{\log\left(4\frac{r_M}{r_1}\right)}\right).$$

Using the right bound in (15) we infer that

$$\sigma_{2i} \leq C\|\alpha\|_{\ell^2(\mathbb{R})} \exp\left(-\frac{\pi^2 i}{\log(r_M) - \log\left(\frac{r_1}{4}\right)}\right) \leq C'\|\alpha\|_{\ell^2(\mathbb{R})} \exp\left(-\frac{\pi^2 i}{2\log(r_M)}\right). \quad ■$$

Remark A.1. When $m \approx \mu M$ with $0 < \mu \leq 1$ we have that

$$\sigma_m \leq C\|\alpha\|_{\ell^2(\mathbb{R})} \exp\left(-\frac{\pi^2}{2}\frac{\mu M}{\log(r_M)}\right).$$

These singular values decrease toward zero exponentially fast for large M (*and large* m).

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