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Karhunen-Loève's Series Truncation for Bivariate Functions

M. Azaïez* F. Ben Belgacem†

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Abstract

Karhunen-Loève's decompositions (KLD) or the proper orthogonal decompositions (POD) of bivariate functions are revisited in this work. We investigate the truncation error first for regular functions and try to improve and sharpen bounds found in the literature. However it happens that (KL)-series expansions are in fact more sensitive to the liability of fields to approximate to be well represented by a 'small' sum of products of separated variables functions. We consider this very issue for some interesting fields solutions of partial differential equations such as the transient heat problem and Poisson's equation. The main tool to state approximation bounds is linear algebra. We show how the singular value decomposition underlying the (KL)-expansion is connected to the spectrum of some Gram matrices. Deriving estimates on the truncation error is thus strongly tied to the spectral properties of these Gram matrices which are structured matrices with low displacement ranks.

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1 Introduction

Model Reduction methods developed for data analysis and scientific computing are used as enhancing numerical material in the treatment of dynamical systems. They are among important up-to-date factors in deriving fast and reliable solutions to large scale problems (see [21]). In signal processing for instance, Karhunen-Loève's expansion (KLE) turns out to be a practical procedure for a low dimensional representation of spatiotemporal signals (see [20, 11, 25]). Different communities point at it under different terminologies. It is named the proper orthogonal decomposition (POD) in mechanical computation (see [5]), referred to as the principal components analysis (PCA) in statistics (see [27, 16, 17]) and data analysis or called singular value decomposition (SVD) in linear algebra (see [12]). These are the most known terminologies ; other denominations do exist. A great amount work has been realized and a wide literature has been elaborated on the application of these techniques to reduce computational cost in various areas which proves them tractable to handle many interesting problems. We refer to the papers, manuscripts and lecture notes [27, 15, 10, 19, 33, 30, 28, 26] and references therein. Of course this, and by far, is not an exhaustive list of research touching the subject.

In the other hand side, fewer papers can be found that are specifically devoted to the mathematical analysis of the (KL)-truncation error. We quote for instance [13]. The estimate on the truncation error provided there is mainly fed by the regularity assumptions on the bivariate field under consideration. That bound tells that the error is expected to decay faster for smoother fields. This result is beyond doubt useful, at least because it concerns a large and well identified class of functions. But, the success of a small truncation to produce a good approximation for a given spatiotemporal (bivariate) field has obviously to do with the possibility for that field to be represented by separated time and space functions. This is not necessarily linked to any smoothness properties. Proving error estimates for general functions seems to be out of reach. Stating sharp estimates for some spatiotemporal fields that are solutions of some common parabolic or elliptic partial differential equation appears more affordable. This is the main target of the current work. To start with, the (SVD)-problem underlying the (KL)-expansion is reworded using linear algebra. The advantage is, at least for spatiotemporal functions we are concerned with, that the underlying eigenvalue problem is related to some infinite dimensional structured matrices such as Cauchy or Pick matrices. Their low displacement rank enables one to derive asymptotics for the corresponding eigenvalues, after which we prove the optimal error estimates we aim at.

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 salient properties, in particular its optimality in the sense that it is among all possible expansions the one that capture the largest fraction of the total energy with a given number of modes. Section 3 is to revisit the

error estimate, caused by the truncation of the (KL)-expansion, provided in [13] for regular functions. In a simple context we illustrate how to enhance the methodology followed there in order to improve the final convergence rate. In section 4, we investigate the truncation error for the solutions of two transient heat equations. In the first one, the temperature field is the one obtained by the conduction of a given initial state while the second temperature field originates from the heat equation where the heating source is given by a time space separated functions. Next, in Section 5 we study the (KL)-approximation of some potential obtained as the solution of Poisson's equation. In the Appendix, asymptotics of some useful Pick matrices are exposed.

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 [2].

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 . It is expressed by

$$\varphi \mapsto B \varphi, \quad (B \varphi)(y) = \int_X T(x, y) \varphi(x) dx. \quad (1)$$

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 $L^2(X)$. It is also an integral operator and is given by

$$v \mapsto B^* v, \quad (B^* v)(x) = \int_Y T(x, y) v(y) dy. \quad (2)$$

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, its kernel K is expressed by

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

We have that $K \in L^2(X \times X)$; A is of course compact. Applying the Hilbert Schmidt theorem enables the diagonalization of A . There exists then 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 , that is

$$A \varphi_m = \lambda_m \varphi_m, \quad \forall m \geq 0. \quad (3)$$

Assume that the sequence $(\lambda_m)_{m \geq 0}$ is positive, which means that B is injective. We retain this option to be focussed on the main ideas we want to expose here while avoiding as much as we can mathematical technicalities. Extension to the general case is readily checked. Hence, 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 $(\varphi_m, v_m, \sigma_m)_{m \geq 0}$ such that $(\varphi_m)_{m \geq 0}$ is an orthonormal basis in $L^2(X)$, $(v_m)_{m \geq 0}$ an orthonormal system in $L^2(Y)$ and $(\sigma_m)_{m \geq 0}$ a sequence of nonnegative real numbers such that*

$$B \varphi_m = \sigma_m v_m, \quad B^* v_m = \sigma_m \varphi_m.$$

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 [9] 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 out of the kernel K a Mercer kernel. Using Mercer's theorem yields the following decomposition (see [22])

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

A direct result is the Karhunen-Loève expansion, currently used in the analysis of stochastic processes (see [3, 34]). It is more commonly known under the Proper Orthogonal Decomposition terminology and the related acronym is (POD) in the partial differential equations literature.

Corollary 2.2 *The following expansion holds*

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

Remark 2.2 *Considering the functions $w_m = \sigma_m v_m$, the Karhunen-Loève decomposition may be put under the following form*

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

The system $(w_m)_{m \geq 0}$ is orthogonal with

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

The quality of the function T to be accurately represented by truncated 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). The orthogonality produces the following estimate*

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

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 used. When it is applied for the representation of 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 [24]).*

3 Truncation error

A brief discussion is conducted here about the approximation error. We focus on some particular situations to provide the key-ideas for a relevant study 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

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

We refer for instance to [20, 11, 31] 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 realizes 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 [13]. We noticed that the result stated there lacks optimality. This is the reason why we expose briefly the way to improve that proof. Our choice is thus to handle a simple case to give clues to successfully achieve such an improvement.

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

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

The functions $(\tau_k)_{k \geq 0}$ are given by

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

These are preliminaries to state an estimate of the KL-approximation error. 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

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

Calling for the abstract estimate (5), we have that

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

Observe that $S_M(\cdot, y)$ is obtained by the orthogonal projection of $T(\cdot, y)$ on the space of polynomial with degree $\leq M$. First, let j be an integer. Consider that $T \in H^j(I, L^2(Y))$, then by Fubini theorem we obtain that $\partial_x^{(j)} T \in L^2(I \times Y)$. Following the proof developed in [6, Chap. III, Theorem 1.2] we derive that

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

We emphasize on the fact that C does not depend on y . Switching to the square power and integrating on the variable $y \in Y$ completes the proof for $\tau = j$. The extension to the fractionary Sobolev spaces $H^\tau(I, L^2(Y))$, with $\tau \in \mathbb{R}_+$, is achieved by Hilbertian interpolation in the same way as [6, Chap. III]. ■

Remark 3.1 *The convergence rate given in [13] is not the best one could obtain. Applied to our case, the bound obtained by [13, Theorem 3.4] would be $C_T M^{1/2-\tau}$. This suffers from a lack of optimality because of the extra-term $M^{1/2}$. The proof proposed in there sounds biased somehow because it relies on the estimates of the singular values of the integral operator B . This is not the right road to be taken. The proof should be tackled directly, through estimate (5) and using the tensorized argument exposed in [6, Chap. III, Théorème 2.4] and employed here.*

Remark 3.2 *The bound obtained in Proposition 3.1 could not be substantially improved for general functions. To be convinced, consider the case $Y = I$ and let us have a look at the function*

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

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

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

Evaluating the approximation error yields the following bound

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

This is close to the worst bound predicted by the proposition which is M^{-1} . Proceeding like in [6, Chap. III, Remark 1.4]. It would be possible to construct an accurate example to illustrate that result in Proposition 3.1 can not 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. Sometimes, we need in fact to look closely at the singular values $(\sigma_m)_{m \geq 0}$ of the operator B or equivalently at the eigenvalues $(\lambda_m)_{m \geq 0}$ of the operator A . It can be checked out that these $(\lambda_m)_{m \geq 0}$ are the eigenvalues of the Gram matrix

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

Their magnitude are likely dependent on the size of the entries of \mathcal{G} . This has to do with the smoothness of T . The point we focus on in the subsequent is the influence of the geometry of the family $(\tau_k)_{k \geq 0}$, in particular 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 [8]).

Remark 3.3 *Regarding this specific orthogonality point, if for instance the functions $(\tau_k)_{k \geq 0}$ are orthogonal then Gram's matrix \mathcal{G} is diagonal and according to Remark 3.2, the sum (6) is nothing else than the Karhunen-Loève expansion and the result of Proposition 3.1 can not be improved.*

4 Transient temperature

We investigate two examples picked up from transient heat transfer. Writing down the temperature field as a Fourier series is as old as the closed expression of the solutions to the heat equation. The infinite Fourier sum enjoys some 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 liable to preserve the main features of the temperature field with high accuracy. The purpose is therefore to illustrate the impact of the orthogonality defect suffered by Fourier expansion of the field T and show how the Karhunen-Loève decomposition brings a better expression regarding the quality of variables separation.

4.1 Heat equation with no source term

We try to be in accordance with current notations of the heat model that provides the function we are working with. We choose therefore to use t instead of y . Assume that $I =]0, \pi[$ and $J =]0, b[$, t is the time variable and x is the space variable. We are thus interested in the heat model. Since we are still concerned by an easy presentation of our analysis. We then choose to present the oneD case although all the subsequent results are readily extended to the higher dimension.

In this example, no heating source is present in the heat problem other than the initial state. The related value equation consists hence of: *finding a temperature field T such that*

$$\begin{aligned} \partial_t T - \gamma \partial_x^2 T + \beta T &= 0, & \text{in } I \times J, \\ T(0, \cdot) = T(\pi, \cdot) &= 0, & \text{in } J \\ T(\cdot, 0) &= a(\cdot), & \text{in } I. \end{aligned}$$

The conduction parameter is γ and the heat transfer coefficient is β . They are chosen constant only for simplicity. As will be seen none of tools used here is specific to the case of constant parameters. Hence, the whole analysis developed in the subsequent is valid as well for space varying parameters. The temperature field, solution of this problem can be defined by the infinite Fourier sum

$$T(x, t) = \sum_{m \geq 1} a_m e^{-r_m t} \sin(mx), \quad \forall (x, t) \in I \times J. \quad (7)$$

The sequence $(r_m)_{m \geq 1}$ is dependent upon γ and β , it is given as $r_m = \gamma m^2 + \beta$. The Fourier coefficients $(a_m)_{m \geq 1}$ of the function a are square summable ($\in \ell^2(\mathbb{R})$). This implies that $T \in L^2(I \times J)$ with a zero mean-value with respect to the variable x . Furthermore, it is easily seen that

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

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

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

This is far from being satisfactory. The geometry of the system $(e^{-r_m t})_{m \geq 1}$ will play an important role in enhancing the estimate. This system suffers from a high discrepancy to the orthogonality. It is in fact almost linearly dependent (see [32]). We are going to carry out analytical computations to find out how to strongly improve that approximation result by taking advantage of the singular value decomposition. We start by the calculation of the kernel K related to A . It is given by

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

Now, we expand the function φ as follows

$$\varphi(x) = \sum_{m \geq 1} f_m \sin(mx), \quad \forall x \in I.$$

After replacing in the eigenvalue equation (3), there comes out

$$\frac{2}{\pi} \sum_{k \geq 1} \left(\sum_{m \geq 1} a_k \frac{1 - e^{-(r_m + r_k)b}}{r_m + r_k} a_m f_m \right) \sin(kx) = \lambda \sum_{k \geq 1} f_k \sin(kx).$$

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

$$\mathcal{G}\varphi = \lambda\varphi. \tag{8}$$

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

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

The coefficients of the vector φ are $(f_m)_{m \geq 1}$. The matrix \mathcal{C}_b is symmetric and positive definite. In turn, 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 towards. We refer to [4] and postpone a detailed study of this matrix. This analysis is based on several notions for linear algebra such as Cauchy-like displacement operators, displacement rank, Sylvester-Lyapunov equation, \dots , etc.

¹We dropped the factor $\frac{2}{\pi}$.

To have an immediate idea about the spectral features of the Gram matrix, one may have a glance at \mathcal{C}_∞ ($b = \infty$) (see [7]). This matrix is of Cauchy type and so are all its principal sub-matrices. Their determinants can hence be calculated explicitly. According to [7], the principal sub-determinant with (large) order M_∞ of \mathcal{C}_∞ is given by

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

This determinant decays tremendously fast towards zero for growing M_∞ . This may be an indication that the eigenvalues of \mathcal{C}_∞ decrease rapidly towards zero.

4.2 Influence of a separated source term

We consider the case where a heating source is operating. The shape of the source S is particular. It is represented by a separated function on t and x so that $S = a \otimes \theta$. One hopes that the temperature field shows a strong capacity to be represented by as sum of separated functions. This expectation is true but proving it is not that easy. This is our purpose here. The heat model to handle is the following : *find a temperature field T such that*

$$\begin{aligned} \partial_t T - \gamma \partial_x^2 T + \beta T &= S, & \text{in } I \times J, \\ T(0, \cdot) = T(\pi, \cdot) &= 0, & \text{in } J \\ T(\cdot, 0) &= 0, & \text{in } I. \end{aligned}$$

After carrying out Fourier calculations we come up with the following temperature

$$T(x, t) = \sum_{m \geq 1} a_m \left(\int_{(0,t)} \theta(s) e^{-r_m(t-s)} ds \right) \sin(mx), \quad \forall (x, t) \in I \times J.$$

The sequence $(a_m)_{m \geq 1}$ is for Fourier's coefficient for f . Straightforward integral computations yields the following expression for the Mercer kernel K ,

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

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

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

That the Mercer kernel is explicated, the next point is the determination of the eigenvalues of the operator A . Based on the arguments developed in the previous example, we can reword the eigenvalue problem (3) under an algebraic form similar to (8). 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 Section 6. It can be checked that \mathcal{G} satisfies the Lyapunov equation with the same Cauchy-like displacement operator that is

$$\mathcal{R}\mathcal{G} + \mathcal{G}\mathcal{R} = ae^T + ea^T + dd^T. \quad (9)$$

The entries of vectors e and d are given by

$$e_m = \frac{a_m}{2} \int_J \int_J \theta(s) \theta(\tau) e^{-r_m |\tau - s|} ds d\tau \quad d_m = a_m \int_J \theta(s) e^{-r_k (b - s)} ds.$$

The displacement rank of equation (9) is low it is equal to three. Reproducing the proof in Section 6 yields the following result

Proposition 4.1 *Assume that $a_m = 0, \forall m \geq M$ for a large integer M . The following estimate on the singular values of B holds*

$$\sigma_{3m} \leq C(a, \theta) \exp\left(-\frac{\pi^2 m}{2 \log(r_M)}\right), \quad 1 \leq m \leq [(M - 2)/3].$$

Remark 4.1 *Results by Proposition 4.1 predicts that the singular values of the integral operator B decreases speedily towards zero. In case it is really there, the log term we see in the bound may slow down the decaying. 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 the extra log-term is probably there only because we were not able to produce an efficient technical proof to get rid of it.*

4.3 Numerics

To support 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

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

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 stiffness of the representative curve of $a(\cdot)$ at the vicinity of $x = 0$ suggests that it contains a singularity there.

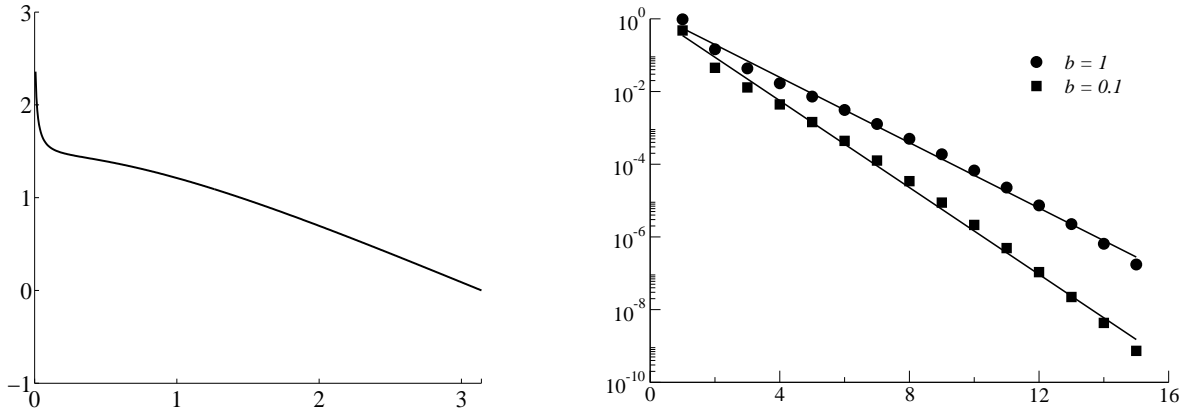


Figure 1: The initial temperature a (left). Singular values for $b = 1, b = 0.1$ (right).

The non-vanishing part of the the Gram matrix \mathcal{G} is thus the principal block of dimension M_∞ ,

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

All the other entries are zeroes. 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 sounds in accordance with the analysis prediction. The singular values sequence decreases toward zero speedily. 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 [6]. Computations are run with the time step equal to $\delta t = 10^{-2}$ and the polynomial degree is fixed to $N = 64$. 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 does not exceed $3/2$. The aim we pursue 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 aptitude to separated representation.

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

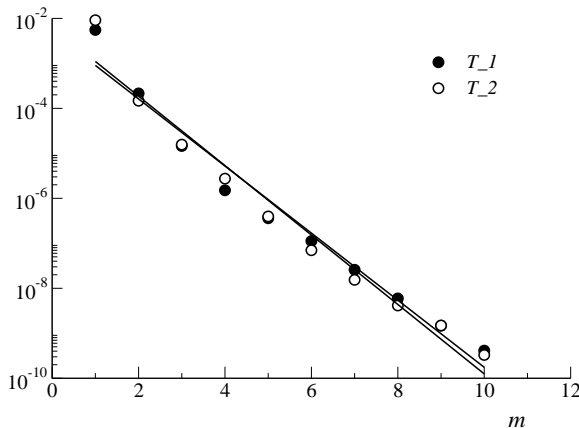


Figure 2: Singular values for T_1 and T_2 .

In the last example with the transient heat transfer, the source term contains a strong coupling of both variables t and x . It is defined as

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

We guess that the solution T_3 will show a weak ability to be represented by a sum of separated

²The procedure `dsyevd` from LAPACK is called.

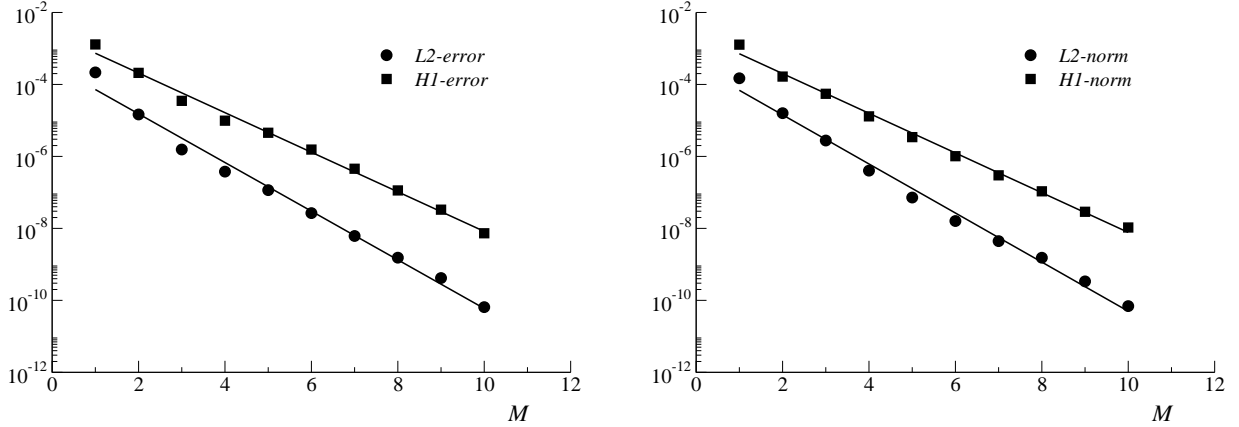


Figure 3: Truncation errors versus the cut-off M , for T_1 and T_2 .

functions. Thus, the singular values of the integral B operator are expected to decay slowly, at least not exponentially. They are plotted in Fig. 4 in a *full logarithmic scale*. The decaying rate seems to be polynomial. Indeed, after the eliminating the first singular value, the polynomial regression tells us that those $(\sigma_m)_m$ decreases like $m^{-4.9}$. Now, according the estimate (4), the L^2 -norm of the error is expected to behave as

$$\|T - T_M\|_{L^2(I \times J)} \leq C \sqrt{\sum_{m \geq M+1} (\sigma_m)^2} \approx C \sqrt{\sum_{m \geq M+1} m^{-9.8}} \approx CM^{-4.4}.$$

The convergence rate of the L^2 -truncation error obtained as the slope of the linear regression in the right diagram in Fig. 3 equals $M^{-4.10}$. Both expected 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 $M^{3.19}$. The temperature field T_3 is less inclined than T_1 and T_2 , to be represented by separated functions. Notice that computations were run after a variational Euler scheme/Legendre spectral method has been conducted.

5 Potentials from Poisson's equation

We investigate here the case of some particular potentials considered in [8, Chap. 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

$$V(x, y) = \sum_{k \geq 1} \sum_{m \geq 1} \frac{f_{km}}{k^2 + m^2} \sin(kx) \sin(my), \quad \forall (x, y) \in I \times I. \quad (10)$$

The doubly indexed sequence of reals $(f_{km})_{k, m \geq 1}$ 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

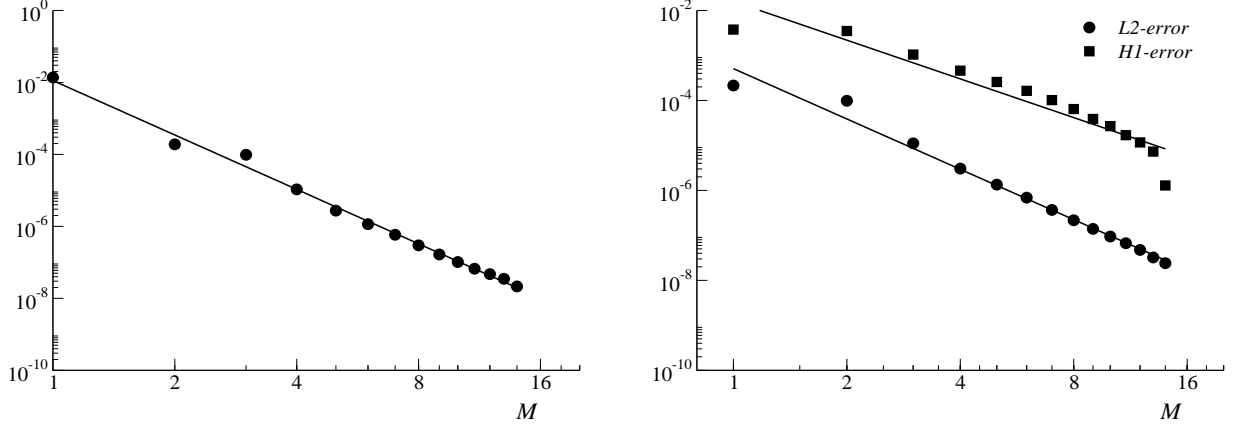


Figure 4: Singular values for T_3 (left). Truncation errors versus M (right).

the Poisson equation set in the square $I \times I$ with homogeneous Dirichlet condition and the function f being the source datum : *find a potential field V such that*

$$\begin{aligned} -\Delta V &= f & \text{in } I \times I, \\ V &= 0 & \text{in } \partial(I \times I). \end{aligned}$$

Analytical computations may be carried out here 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 (10), and all calculations achieved, the expression we obtain is

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

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

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

\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 $k, m, \ell \geq 1$,

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

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 we accept the notations abuse and 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. To be complete with this particular case, we stress on the fact that the potential V has a moderate Sobolev regularity because of the corner singularities (see [14]). Indeed, $V \in H^\tau(I \times I)$ only for $\tau < 3$. Based in 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 5. A semi-logarithmic scale is adopted. The decaying rate so as the convergence rates of the errors seem to be at least exponential.

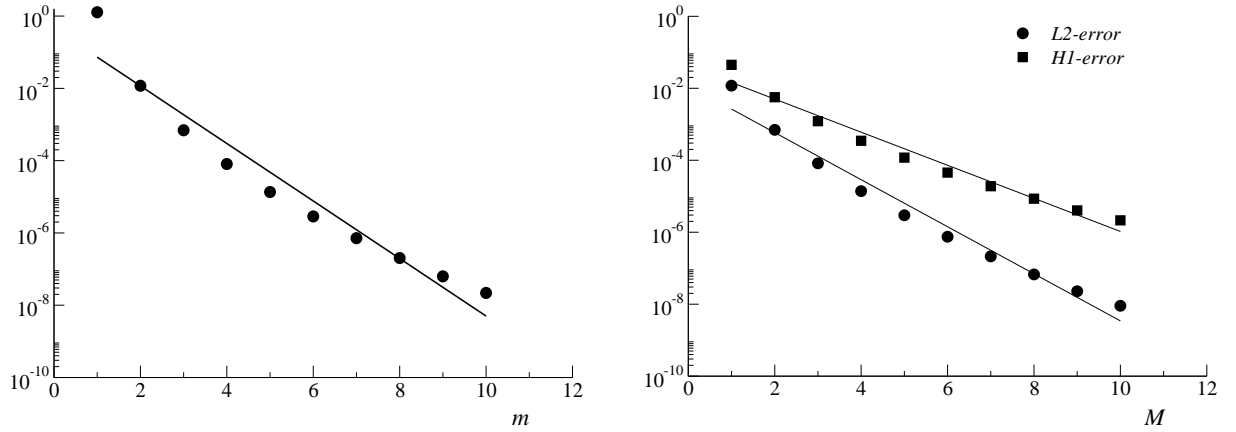


Figure 5: Singular values for V (left). Truncation errors (right).

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

$$V(x, y) = \frac{1}{\pi} \sum_{m \geq 1} \frac{1}{m^2} \sin(mx) \sin(my), \quad \forall (x, y) \in I \times I. \quad (11)$$

This new potential V has in fact lesser 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 (11) 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

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

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

By the way, 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

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

The sequence of the singular values $(\sigma_m)_{m \geq 1}$ coincides with the diagonal coefficients. It decreases slowly towards 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. 6 depicts 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.

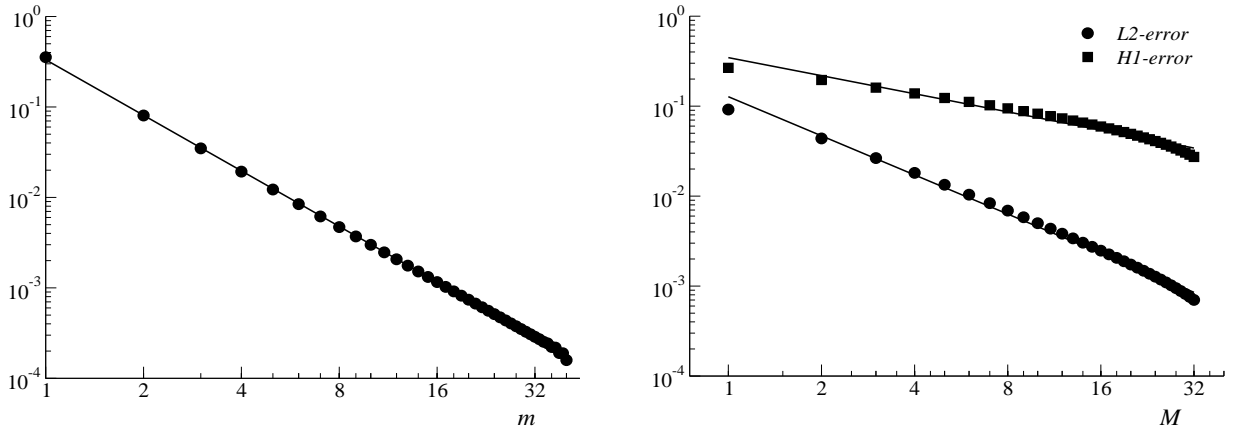


Figure 6: Singular values for V (left). Truncation errors (right)

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 firsts arise as solutions of transient heat equations and the others are potentials fulfilling the Poisson boundary value problem. The results shown are in accordance with numerical trends observed in many works. The truncation error decreases exponentially fast with respect to the number of (KL)-modes retained. The method followed here is mainly algebraic and is based on the asymptotics of the spectra of some symmetric structured matrices.

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

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

The matrix \mathcal{G} is symmetric and non-negative. It 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 $a = (a_k)_{k \geq 1}$ and $a' = (a_k e^{-r_k b})_{k \geq 1}$. It is readily checked that the matrix \mathcal{G} satisfies the Lyapunov equation

$$\mathcal{R}\mathcal{G} + \mathcal{G}\mathcal{R} = aa^T - (a')(a')^T. \quad (12)$$

This equation is related to the notion of displacement operators (see [18]). 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 $aa^T - (a')(a')^T$ is called the displacement rank of equation (12). 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} are strongly connected to the properties of the displacement operator and by then on the diagonal matrix \mathcal{R} and to the displacement rank of (12). Bounds will be derived after applying results that have been surveyed in [29, 2006]. The following result holds

Proposition 6.1 *We have that*

$$\sigma_1 \leq \|a\|_{\ell^2(\mathbb{R})} \left(\sum_{m \geq 1} \frac{1}{(r_1 + r_m)^2} \right)^{1/4}. \quad (13)$$

Proof: The bound on the largest eigenvalue $\lambda_1 = (\sigma_1)^2$ of \mathcal{G} may be established owing to the Gershgorin-Hadamard circle theorem (see [23, Chapter 8]),

$$\lambda_1 \leq \max_{1 \leq k \leq M} \sum_{1 \leq m \leq M} a_k a_m \frac{1 - e^{-(r_k+r_m)b}}{r_k + r_m}.$$

We deduce by Cauchy-Schwarz inequality that

$$\lambda_1 \leq \max_{1 \leq k \leq M} |a_k| \left(\sum_{1 \leq m \leq M} (a_m)^2 \right)^{1/2} \left(\sum_{1 \leq m \leq M} \frac{1}{(r_1 + r_m)^2} \right)^{1/2}. \quad (14)$$

We infer that

$$\lambda_1 \leq \|a\|_{\ell^2(\mathbb{R})}^2 \max_{1 \leq k \leq M} \left(\sum_{1 \leq m \leq M} \frac{1}{(r_k + r_m)^2} \right)^{1/2} = \|a\|_{\ell^2(\mathbb{R})}^2 \left(\sum_{1 \leq m \leq M} \frac{1}{(r_1 + r_m)^2} \right)^{1/2}.$$

The bound (13) is established after switching to the square roots. ■

Proposition 6.2 *Assume M be large enough. The following bound holds*

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

Proof: Let us observe first that the displacement rank of the Lyapunov equation (12) is two. Calling for Theorem 2.1.1 of [29, pages 39-40] yields the following bound

$$\frac{\lambda_{2i}}{\lambda_1} \leq C \exp\left(-\frac{\pi^2 i}{\log(4\kappa(\mathcal{R}))}\right). \quad (15)$$

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

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

Using the right bound in (14) we infer that

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

The proof is complete. ■

Remark 6.1 *When $k \approx \eta M$ with $0 < \eta \leq 1$ we have that*

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

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

Remark 6.2 *A perfect estimate would be derived if one gets rid from the log-term $\log(r_M)$ in (15). To our opinion, it should be possible to remove that extra-term by improving the mathematical techniques to obtain optimal bounds for symmetric Cauchy or Pick matrices.*

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