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parametric and stochastic Elliptic PDEs

by

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Abstract

We investigate the convergence rate of approximations by finite sums of rank-1 tensors of solutions of multi-parametric elliptic PDEs. Such PDEs arise, for example, in the parametric, deterministic reformulation of elliptic PDEs with random field inputs, based for example, on the M -term truncated Karhunen-Loève expansion.

Our approach could be regarded as either a class of compressed approximations of these solution or as a new class of iterative elliptic problem solvers for high dimensional, parametric, elliptic PDEs providing linear scaling complexity in the dimension M of the parameter space.

It is based on rank-reduced, tensor-formatted separable approximations of the high-dimensional tensors and matrices involved in the iterative process, combined with the use of spectrally equivalent low-rank tensor-structured preconditioners to the parametric matrices resulting from a Finite Element discretization of the high-dimensional parametric, deterministic problems.

Numerical illustrations for the M -dimensional parametric elliptic PDEs resulting from sPDEs on parameter spaces of dimensions $M \leq 100$ indicate that the gain from employing low-rank tensor-structured matrix formats in the numerical solution of such problems might be substantial.

AMS Subject Classification: 65F30, 65F50, 65N35, 65F10

Key words: elliptic operators, stochastic PDEs, the Karhunen-Loève expansion, polynomial chaos, separable approximation, Kronecker-product matrix approximations, high-order tensors, preconditioners, tensor-truncated iteration.

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1 Introduction

Recent advances in the numerical methods based on separation of variables applied to the functions and operators in \mathbb{R}^d , lead to the natural idea of solving multi-dimensional boundary value and spectral problems in tensor-product data formats. This idea was for the first time formulated in [2] in a very general framework. Tensor-structured techniques in higher dimensions [7, 13, 15, 23, 26] have already demonstrated their solid potential in electronic structure calculations [3, 12, 23, 24, 25], in PDEs with random input [34, 37, 35, 4], and in machine learning [1].

In the present paper, we introduce the low rank tensor approximation method for solving the deterministic parametric elliptic equations in a high (possibly infinite) dimensional parameter space, arising as a projection of the stochastic PDE via a *truncated M -term Karhunen-Loève expansion*. We consider a class of model elliptic problems characterized by the additive dependence of the equation coefficients on the multivariate parameter, corresponding to a random field that is linear in the random variable. Exploiting sparsity in the solutions polynomial chaos expansion leads to superalgebraic (subexponential) convergence rates of Galerkin as well as of collocation approximations in terms of the number N of deterministic diffusion problems to be solved, [37, 4] in the case that the Karhunen-Loève expansion of the input random field converges exponentially and to algebraic convergence rates of best N -term polynomial approximations of the parametric solution [6]. N -term truncated polynomial chaos expansions are separable expansions. Therefore, we can adapt the concept of rank structured approximation to tensor products of solution spaces in the physical domain D and to multi-dimensional parametric spaces. We show that the FEM-Galerkin approximation in a tensor-product basis allows for approximate low tensor-rank representations of arising stiffness matrices and right-hand sides. The principal idea of our approach is the iterative solution of a single coupled system of discrete, multiparametric elliptic equations projected onto the nonlinear manifold of low rank tensor-structured vectors. The numerical cost of the matrix-vector multiplication in our setting scales linear in M , and at most quadratically in the univariate discrete problem size. In this way, the use of adaptive low rank tensor formats allows to avoid the exponential growth in M , the dimension of the parameterspace, increasing complexity of tensor approximations while, at the same time, preserving the convergence rate of the stochastic Galerkin approximations.

To enhance the convergence of the global solver, we propose the preconditioned block Jacobi-type iteration accomplished with the rank optimization at each iterative step. Our basic preconditioner is constructed using the tensor-product approximation to the parametric elliptic operator inverse with the spatially homogeneous random coefficients.

In the case of constant stochastic coefficients the method is proved to have almost linear complexity in the univariate discrete problem size, as well as in the dimension of stochastic variable, M . In general, it leads to algebraic complexity $O(M\varepsilon^{-q})$ with respect to the model accuracy $\varepsilon > 0$, where $q > 0$ is some fixed constant independent on M . In summary, this asymptotic performance is achieved by combining the following ingredients:

- low-rank tensor-structured matrix formats used for the separable representation of all multidimensional matrices and vectors involved,
- efficient rank optimisation algorithms via tensor-structured nonlinear approximation,

- application of spectrally close rank-structured preconditioners to the FEM-Galerkin matrix leaving in higher dimensional space.

The rest of the paper is organized as follows. In §2, we set up the problem, and recall the regularity results for the solution of the initial equation in terms of analyticity domain in parametric space [35]. We also present the definitions of tensor structured vector- and matrix-formats to be used in the paper. In §3, we discuss the tensor-product FEM, describe the basic low tensor rank preconditioner, prove its spectral equivalence, and then introduce the respective iterative solvers with adaptive rank optimization via best R -term nonlinear approximation. In §4, we first present some numerical illustrations for the case of constant coefficients in a high-dimensional setting, which provide the base for efficient preconditioning. Second, we give numerical examples with variable stochastic coefficients, corresponding to random fields that are linear in the random variable. We investigate the case of both polynomial and exponential decay of stochastic coefficients. In §5, we formulate the preliminary conclusions.

2 High-Dimensional Parametric Elliptic Problem

2.1 Strong formulation

We consider parametric, elliptic problems which are posed in the physical domain $D := (0, 1)^{d_0}$ of dimension $d_0 = 1, 2, 3$, and which depend on a vector of M parameters which take values in the hypercube in the M -dimensional parametric space $\Gamma := (-1, 1)^M \equiv I^M$, $M \in \mathbb{N}_+$. To formulate the problems, we introduce the tensor-product Hilbert space (cf. [32])

$$V := V_y \otimes V_x \quad \text{with} \quad V_y := L^2(\Gamma) = \bigotimes_{m=1}^M L^2(I), \quad V_x := H_0^1(D).$$

We are given a parametric elliptic operator

$$\mathcal{A}(y) := -\operatorname{div}_x (a(y, x) \operatorname{grad}_x) \quad \text{and} \quad f \in L^2(D), \quad y \in \Gamma$$

where the coefficient $a(y, x)$ is a smooth function of $x \in D$ and the parameter vector $y = (y_1, \dots, y_M) \in \Gamma$ with a possibly very large number M of parameters. We are interested in the efficient numerical solution of the parametric elliptic problem: for every $y \in \Gamma$, find $u_M \in V$, such that

$$\mathcal{A}u_M(y, x) = f(x) \text{ in } D, \quad u_M(y, x) = 0 \text{ on } \partial D. \quad (2.1)$$

In this problem setting the dimension M of the parametric space corresponds to the truncation parameter in the Karhunen-Loève expansion (see, e.g., [35]). In discretizations of diffusion problems with random inputs, the dimension M of the parameter space could become arbitrarily large.

2.2 The unique solvability of weak equation

We consider the class of problems, with the coefficient function defined by

$$a_M(y, x) := a_0(x) + a_y(y, x), \quad \text{where } a_y(y, x) = \sum_{m=1}^M a_m(x)y_m, \quad (2.2)$$

with $a_m \in L^\infty(D)$, $m = 1, \dots, M$. Hence, for $y \in \Gamma$, one can introduce the associated parametric bilinear form in the physical space V_x ,

$$A(u, v) := \langle \mathcal{A}u, v \rangle_{L^2(D)} = \int_D a_M(y, x) \nabla_x u \cdot \nabla_x v dx \quad \forall u, v \in V_x,$$

so that we can use the respective to (2.2) additive splitting

$$A(u, v) = A_0(u, v) + A_y(u, v) \quad \forall u, v \in V_x,$$

where A_0 does not depend on $y \in \Gamma$. Concerning the coefficient function $a_M(y, x)$, we assume that there exists $a_{min} > 0$, such that

1. $a_{min} \leq a_0(x) < \infty$,
2. $\left| \sum_{m=1}^M a_m(x)y_m \right| < \gamma a_{min}$ with $\gamma < 1$, and for $|y_m| < 1$ ($m = 1, \dots, M$).

Conditions 1) - 2) imply the strong ellipticity of the problem (2.1) uniformly in y , i.e.,

$$a_M(y, x) \geq (1 - \gamma)a_{min} > 0. \quad (2.3)$$

Hence, under assumptions 1) - 2), we have the unique solvability for the corresponding weak formulation: for any $f \in H^{-1}(D)$ and for any $y \in \Gamma$, there exists a unique solution $u_M(y, \cdot) \in H_0^1(D)$ of the problem: Find $u_M \in V_x$, such that

$$\text{Find } u_M \in V_x, \text{ such that } A(u_M, v) = \int_D f(x)v(x)dx \quad \forall v \in V_x. \quad (2.4)$$

The *parametric weak equation* (2.4) can be reformulated as the variational equation in the tensor-product Hilbert space V . Introducing the respective bilinear form

$$A_M(u, v) := \int_\Gamma \int_D a_M(y, x) \nabla_x u \cdot \nabla_x v dx dy \quad \forall u, v \in V,$$

we arrive at the following variational problem : Find $u_M \in V$, such that

$$A_M(u_M, v) = \int_\Gamma \int_D f(x)v(y, x) dx dy =: b_M(v) \quad \forall v \in V. \quad (2.5)$$

Lemma 2.1 *The equation (2.5) is uniquely solvable in V .*

Proof. Using the strong ellipticity condition (2.3) we obtain

$$A_M(v, v) := \int_\Gamma \int_D a_M(y, x) \nabla_x v \cdot \nabla_x v dx dy \geq (1 - \gamma)a_{min} \int_\Gamma \|v(y, \cdot)\|_{V_x}^2 dy,$$

which proves the strong ellipticity of the bilinear form $A_M : V \times V \rightarrow \mathbb{R}$. Conditions 1) - 2) also imply the continuity of A_M . The result then follows. \blacksquare

We discretize the parametric equation (2.5) by Galerkin FEM in both domains, Γ and D . In order to assess the convergence of these methods, we first review some results on regularity of the solution.

2.3 Regularity

In [37] it is proved that the weak solution $u(y, \cdot) \in H_0^1(D)$ is analytic as a map

$$y \mapsto u(y, \cdot) \in H_0^1(D) \quad \text{from } \Gamma \text{ to } H_0^1(D).$$

A precise analysis with quantitative bounds on the size of the domain of analyticity is based on a-priori assumptions on the decay of the coefficients in (2.2). We distinguish two basic cases of coefficient decay:

1. Exponential decay (see [37], (4.5)):

$$\rho_m := \|a_m\|_{L^\infty(D)} \leq C_0 \exp(-C_1 m^{1/d_0}) \quad \forall m \in \mathbb{N}_+. \quad (2.6)$$

Note that the sequence $\rho = (\rho_m)_{m=1}^\infty$ in (2.6) belongs to $\ell^p(\mathbb{N})$ for every $p > 0$.

2. Algebraic decay (see e.g. [6, 5]): there is a constant $s > 0$ such that in the coefficient bound

$$\rho_m := \|a_m\|_{L^\infty(D)} \leq C_0 m^{-s/d_0} \quad \forall m \in \mathbb{N}_+. \quad (2.7)$$

Note that the sequence $\rho = (\rho_m)_{m=1}^\infty$ in (2.7) belongs to $\ell^p(\mathbb{N})$ for every $p > d_0/s$.

Based on the coefficient decay (2.6) it was proved in [37] that the domain of analyticity of the solution u of (2.1) as a function of y_m , increases exponentially in size as $m \nearrow \infty$.

Explicit bounds on all derivatives of u with respect to y_m which are applicable in either case 1. and 2. are given by the following statement.

Proposition 2.2 ([37]) *If $u = u_M(y, \cdot)$ solves (2.1), then assumption (2.6) implies*

$$\|\partial_y^\alpha u_M(y, \cdot)\|_{H_0^1(D)} \leq \left(C_a^{|\alpha|} \cdot |\alpha|! \cdot \prod_{m=1}^M \rho_m^{\alpha_m} \right) \quad (2.8)$$

$\forall y \in I^M, \forall \alpha \in \mathbb{N}_0^M$, and for all M large enough.

A class of parametric, elliptic PDEs with polynomial decay of coefficients a_m is specified by the algebraic rate of decay $s > 0$ in the coefficient bound as in (2.7).

Based on assumption (2.6) and on Proposition 2.2 it is shown in [6] that there exists a sequence $\{\Sigma_{M,N}\}_{N=1}^\infty \subset \mathbb{N}_0^M$ of index sets of cardinality not exceeding N and corresponding so-called *best N -term polynomial chaos approximations* $u_{M,N}(y, \cdot)$ being linear combinations of monomials y^α , $\alpha \in \Sigma_{M,N}$, with coefficient $u_\alpha \in V_x$, which converge algebraically to u_M at an algebraic rate $r(s)$. Moreover it was shown in [37] for case 1. that there exists a sequence $\{u_{\Sigma_M}\}_{M=1}^\infty$ of tensor-product approximations of u_M specified by monomials $y^\alpha = y_1^{\alpha_1} y_2^{\alpha_2} \dots$ of degrees α_m of magnitude at most $O(M^\kappa)$ ($m = 1, \dots, M$) of the form

$$u_{\Sigma_M} := \sum_{\alpha \in \Sigma_M} \Phi_\alpha(x) y^\alpha, \quad \Phi_\alpha \in V_x, \quad (2.9)$$

such that, as $M \rightarrow \infty$,

$$\|u_M - u_{\Sigma_M}\|_{L^\infty(I^M, H_0^1(D))} \leq C e^{-\beta M^\kappa}, \quad \kappa = 1/d_0,$$

where $\beta, C > 0$ do not depend on M . Furthermore, the cardinality R of the index sets Σ_M satisfies the bound

$$R := \#\Sigma_M \leq C_1 e^{\beta_1 M^{\kappa/(\kappa+1)} \log(M+2)}, \quad (2.10)$$

where $\beta_1, C_1 > 0$ are independent of M (see [37], Corollary 4.16).

In case 2., it was shown in [6] that there exists a sequence $\{\Sigma_M\}_{M=1}^\infty$ of sets of finitely supported multiindices $\alpha \in \mathbb{N}_0^{\mathbb{N}}$ of cardinality R not exceeding M and corresponding separable approximations

$$u_{\Sigma_M} = \sum_{\alpha \in \Sigma_M} \Phi_\alpha(x) L_{\alpha_1}(y_1) L_{\alpha_2}(y_2) \dots \quad \Phi_\alpha \in V_x$$

where $L_{\alpha_1}(y_1) L_{\alpha_2}(y_2) \dots$ denote finite products of Legendre Polynomials of degrees α_m . The products are finite due to the multi-index set Σ_M being ‘‘finitely supported’’, i.e. $\forall \alpha \in \Sigma_M$, $|\alpha|_1 < \infty$, such that the algebraic decay (2.7) implies the error bound

$$\|u_M - u_{\Sigma_M}\|_{L^2(I^M, H_0^1(D))} \leq C(r) R^{-\theta}, \quad 0 < \theta < \frac{s}{d} - \frac{1}{2} \quad (2.11)$$

as $R := \#\Sigma_M \rightarrow \infty$, where $C(r)$ is independent of M .

2.4 Tensor-structured Approximations

We use the above approximation results to infer convergence rates of several formatted matrix tensor approximations of the solution u_M . Importantly, there are nonlinear rank truncation algorithms which operate on several formatted matrix/vector classes and ensure certain quasioptimality properties of the reduced rank-structured tensor approximations. Combining the above approximation bounds and observing that ‘‘polynomial chaos’’ type approximations such as (2.9) are particular, separated low rank approximations, the above regularity results allow to infer convergence rates of formatted low tensor rank approximations for several low-rank tensor-structured matrix formats which we recapitulate next.

2.4.1 Tensor Formats for d -dimensional Arrays

Let $\mathbb{H} = H_1 \otimes \dots \otimes H_d$ denote a tensor-product Hilbert space (see [32]), where H_ℓ ($\ell = 1, \dots, d$) is a separable Hilbert space of functions over \mathbb{R}^{m_ℓ} (continuous setting) or over finite/infinite index sets (discrete setting)¹. This implies that each $w \in \mathbb{H}$ can be represented in a unique fashion by (possibly infinite) sums of rank-1 tensors

$$W = \sum_k w_k^{(1)} \otimes w_k^{(2)} \otimes \dots \otimes w_k^{(d)} \quad (w_k^{(\ell)} \in H_\ell).$$

A scalar product in \mathbb{H} which is consistent with the scalar products $\langle \cdot, \cdot \rangle_{H_\ell}$ in the H_ℓ is defined first on rank-1 elements in \mathbb{H} by

$$\langle w^{(1)} \otimes \dots \otimes w^{(d)}, v^{(1)} \otimes \dots \otimes v^{(d)} \rangle := \prod_{\ell=1}^d \langle w^{(\ell)}, v^{(\ell)} \rangle_{H_\ell}.$$

¹For simplicity, we consider here only finite tensor products of $d < \infty$ many factors; we emphasize, however, that all concepts introduced below can be generalized to tensor products of countably many factors and that such countable tensor products do arise in the applications of interest to us.

It is then extended to all of \mathbb{H} by continuity, see, e.g. [32].

A *tensor of order d* is a multidimensional array of data, $I_1 \times \dots \times I_d \rightarrow \mathbb{R}$, considered as an element a tensor-product Hilbert space $\mathbb{H} = \mathbb{R}^{\mathcal{I}}$, $\mathcal{I} = I_1 \times \dots \times I_d$. Its entries take values in \mathbb{R} and are indexed by corresponding multi indices taking values in a Cartesian product of index sets \mathcal{I} . The index sets I_1, \dots, I_d could be finite or infinite, and need not have the same cardinality. For examples, for $d = 2$ and $H_\ell = \mathbb{R}^n$, we obtain order two tensors which coincide with $n \times n$ square matrices of real-valued entries: here, $\mathbb{H} = \mathbb{R}^{n \times n} \simeq \mathbb{R}^{n^2}$.

In the applications we have in mind, the dimension parameter d is related to the truncation parameter M in the separable expansion (2.2) by $d = M + 1$. We write

$$V = [v_{i_1, \dots, i_d} : i_\ell \in I_\ell] \in \mathbb{R}^{\mathcal{I}}, \quad I_\ell = \{1, \dots, n_\ell\}, \quad \ell = 1, \dots, d,$$

to denote a d -th order tensor of finite size \mathbf{n} , where $\mathbf{n} = (n_1, \dots, n_d)$ denotes the d -tuple. A tensor V is an element of the tensor-product Hilbert space $\mathbb{H} = \mathbb{V}_{\mathbf{n}} = \otimes_{\ell=1}^d \mathbb{V}_\ell$ of real-valued d -fold arrays with $\mathbb{V}_\ell = \mathbb{R}^{I_\ell}$, and equipped with the Euclidean *inner product* $\langle \cdot, \cdot \rangle : \mathbb{V}_{\mathbf{n}} \times \mathbb{V}_{\mathbf{n}} \rightarrow \mathbb{R}$ and related Frobenius norm.

To avoid exponential scaling with respect to the dimension parameter d in the standard multilinear algebra, we use approximate representations in certain classes $\mathcal{S} \subset \mathbb{V}_{\mathbf{n}}$ of “rank structured” elements based on sums of rank-1 tensors. In this way, the *outer product* of vectors $t_\ell = \{t_{\ell, i_\ell}\}_{i_\ell \in I_\ell} \in \mathbb{V}_\ell$ ($\ell = 1, \dots, d$) forms the canonical rank-1 tensor

$$T \equiv [t_{\mathbf{i}}]_{\mathbf{i} \in \mathcal{I}} = t_1 \otimes \dots \otimes t_d \in \mathbb{V}_{\mathbf{n}} \quad \text{with entries} \quad t_{\mathbf{i}} = t_{1, i_1} \cdots t_{d, i_d},$$

which requires dn numbers to store it (now linear scaling in the dimension). When $d = 2$, the outer product of two vectors represents a rank-1 matrix.

We next review several data sparse representations of high order tensors based on the Tucker, canonical and the so-called Tensor-Train/Tensor-Chain models commonly used in low rank formatted matrix/vector algebras.

Definition 2.3 *The rank- (r_1, \dots, r_d) Tucker approximation [7] is based on subspaces $\mathbb{T}_{\mathbf{n}} := \otimes_{\ell=1}^d \mathbb{T}_\ell$ of $\mathbb{V}_{\mathbf{n}}$ for certain $\mathbb{T}_\ell \subset \mathbb{V}_\ell$ with $r_\ell := \dim \mathbb{T}_\ell \leq n_\ell$. Given the vector-valued rank parameter $\mathbf{r} = (r_1, \dots, r_d)$, we denote by $\mathcal{T}_{\mathbf{r}, \mathbf{n}}$ (or simply $\mathcal{T}_{\mathbf{r}}$) the subset of tensors in $\mathbb{V}_{\mathbf{n}}$ represented in the so-called Tucker format*

$$T_{(\mathbf{r})} = \sum_{\nu_1=1}^{r_1} \cdots \sum_{\nu_d=1}^{r_d} \beta_{\nu_1, \dots, \nu_d} t_1^{\nu_1} \otimes \dots \otimes t_d^{\nu_d}, \quad (2.12)$$

with some vectors $t_\ell^{\nu_\ell} \in \mathbb{V}_\ell = \mathbb{R}^{I_\ell}$ ($1 \leq \nu_\ell \leq r_\ell$), which form the orthonormal basis of $\mathbb{T}_\ell = \text{span}\{t_\ell^{\nu_\ell}\}_{\nu_\ell=1}^{r_\ell}$ ($\ell = 1, \dots, d$). The parameter $r = \max_\ell \{r_\ell\}$ is called the *maximal Tucker rank*, while the coefficient tensor $\boldsymbol{\beta} = [\beta_{\nu_1, \dots, \nu_d}]$ is known as the *core tensor*.

In many applications we have $r \ll N$, say $r = O(\log N)$ with $N = \max_\ell n_\ell$. In our context, the Tucker format corresponds to the separable approximation (say, via interpolation) by tensor product orthogonal polynomials in y . An adaptive selection process with some optimality properties with respect to the index set Σ_M could be interpreted as a procedure of cancellation of small elements in the Tucker core $\boldsymbol{\beta}$.

Definition 2.4 Given a rank parameter $R \in \mathbb{N}$, we denote by $\mathcal{C}_{R,\mathbf{n}} = \mathcal{C}_R \subset \mathbb{V}_{\mathbf{n}}$ a set of tensors which can be represented in the canonical format

$$U_{(R)} = \sum_{\nu=1}^R \mu_{\nu} u_{\nu}^{\nu} \otimes \dots \otimes u_{\nu}^{\nu}, \quad \mu_{\nu} \in \mathbb{R}, \quad (2.13)$$

with normalized vectors $u_{\ell}^{\nu} \in \mathbb{V}_{\ell}$ ($\ell = 1, \dots, d$). The minimal parameter R in (2.13) is called the rank (or canonical rank) of a tensor.

The rank- \mathbf{r} three-dimensional tensor (TT) format is defined in the spirit of Tucker model, but with essentially reduced ‘‘connectivity’’ constraints (see [28]). As in the case of canonical format it scales linearly in both d and $N = \max\{n_{\ell}\}$. The generalization of the TT-format to the case of ‘‘periodic’’ index chain is given by the following definition (cf. [22]).

Definition 2.5 (Tensor chain format). Given the rank parameter $\mathbf{r} = (r_0, \dots, r_d)$, and the respective index sets $J_{\ell} = \{1, \dots, r_{\ell}\}$ ($\ell = 0, 1, \dots, d$), with the periodicity constraints $J_0 = J_d$. The rank- \mathbf{r} tensor chain (TC) format contains all elements V in $\mathbb{V}_{\mathbf{n}}$ that can be represented as the chain of contracted products of 3-tensors over the d -fold product index set $J := \prod_{\ell=1}^d J_{\ell}$,

$$V = \prod_{\ell=1}^d G^{(\ell)} \quad \text{with given 3-tensors } G^{(\ell)} \in \mathbb{R}^{J_{\ell-1} \times I_{\ell} \times J_{\ell}}. \quad (2.14)$$

Denote this set of tensors by $TC[\mathbf{r}, d] \equiv TC[\mathbf{r}, \mathbf{n}, d] \subset \mathbb{V}_{\mathbf{n}}$. The parameters d, \mathbf{n} can be skipped upon the context.

In the case $J_0 = J_d = \{1\}$ (disconnected chain), this construction coincides with the respective definition of TT format in [28], thus implying $TT[\mathbf{r}, d] \subset TC[\mathbf{r}, d]$.

In the following, we assume that $r_{\ell} = r$ ($\ell = 1, \dots, d$), then the storage requirements for the Tucker (resp. canonical, TC) decomposition is given by $r^d + drN$ (resp. $R + dRN, dr^2N$), where usually $r \ll R$. It is worth to note that $TC[\mathbf{r}, d] \subset \mathcal{C}_{r,\mathbf{n}}$, hence any rank estimate derived for the canonical approximation can be applied to TT/TC formats as well.

Since $\mathcal{T}_{r,\mathbf{n}}, \mathcal{C}_{R,\mathbf{n}}$, and $TC[\mathbf{r}, \mathbf{n}, d]$ are not linear spaces we are led to the *nonlinear approximation* problem

$$A \in \mathcal{S}_0 \subset \mathbb{V}_{\mathbf{n}} : \quad \sigma(A, \mathcal{S}) := \inf_{X \in \mathcal{S}} \|A - X\| \quad (2.15)$$

with $\mathcal{S} \in \{\mathcal{T}_{r,\mathbf{n}}, \mathcal{C}_{R,\mathbf{n}}, TC[\mathbf{r}, \mathbf{n}, d]\}$, where the target tensor A might inherit certain data-sparse structure as follows $\mathcal{S}_0 \in \{\mathbb{V}_{\mathbf{n}}, \mathcal{C}_{R_0,\mathbf{n}}, \mathcal{T}_{r_0,\mathbf{n}}\}$.

In the case $\mathcal{S} = \mathcal{T}_{r,\mathbf{n}}$, the existence of the best approximation element in (2.15) can be proven since it is reduced to maximization over the compact Grassmannian manifold. Moreover, in the case $\mathcal{S} \in \{\mathcal{T}_{r,\mathbf{n}}, TC[\mathbf{r}, \mathbf{n}, d]\}$, the quasi-best approximation can be calculated by using direct QR/SVD-based algorithms described and proved in [8, 23] for the Tucker format, and in [28, 31] for the TT-model. The proof of quasi-optimality for the closely related hierarchical dimension splitting [17] is given in [11].

Notice that in the case of canonical approximation, i.e., $\mathcal{S} = \mathcal{C}_{R,\mathbf{n}}$, the problem (2.15) is equivalent to finding the best R -term approximation with respect to the dictionary of rank-1 tensors. In this case the best R -term approximation might not exist, and, in general, there are no well defined numerical algorithms to compute the quasi-optimal approximation. In our numerical scheme the canonical approximation is calculated approximately by certain heuristic ALS-based algorithm at each step of truncated preconditioned iteration.

2.4.2 Formatted Tensor Representation of Matrices

In the following we also need the Kronecker-product representation of (operators) matrices $\mathbf{A} \in \mathbb{R}^{\mathcal{I} \times \mathcal{I}}$, acting as the linear mapping $\mathbf{A} : \mathbb{V}_{\mathbf{n}} \rightarrow \mathbb{V}_{\mathbf{n}}$. To this end, we introduce, the canonical sum of matrix products (see [15])

$$\mathbf{A} = \sum_{\nu=1}^R \beta_{\nu} A_1^{\nu} \otimes \dots \otimes A_d^{\nu}, \quad \beta_{\nu} \in \mathbb{R}, \quad A_{\ell}^{\nu} \in \mathbb{R}^{n_{\ell} \times n_{\ell}},$$

where matrices A_{ℓ}^{ν} ($\ell = 1, \dots, d$), in turn, may have fully populated, q -diagonal, low rank, hierarchical, Toeplitz or wavelet related structure. We denote this class of matrices as $\mathcal{M}_{R, \mathbf{n}}$. The rank R matrix-vector multiplication of a matrix $\mathbf{A} \in \mathcal{M}_{R, \mathbf{n}}$ with a rank-1 tensor $T \in \mathbb{V}_{\mathbf{n}}$ is defined by the rank- R canonical sum

$$\mathbf{A}T = \sum_{\nu=1}^R \beta_{\nu} A_1^{\nu} t_1 \otimes \dots \otimes A_d^{\nu} t_d \in \mathcal{C}_{R, \mathbf{n}}.$$

The numerical cost of this matrix-vector product depends on the sparsity pattern of the Kronecker factors. In particular, for $O(N)$ -sparse matrices A_{ℓ}^{ν} it amounts to $O(dRN)$, while in the case of fully populated Kronecker factors the cost is bounded by $O(dRN^2)$ (cf. [15]).

The above classes of rank-structured tensors and matrices will be applied in tensor-product Galerkin Finite Element discretizations of the parametric, deterministic problem (2.1).

2.5 Low Rank Tensor Approximations of $u_M(x, y)$

The constant R estimated by (2.10) can be viewed as upper bound on the separation rank of the solution u_M corresponding to the best R -term approximation over the formatted rank decompositions with fixed number of terms (cf. the canonical model and related nonlinear approximation problem).

Though the adapted index set Σ_M mentioned above does not have tensor product structure, it can be embedded into the product index set $\Sigma_M \subset \mathcal{J}^M$ with $\mathcal{J} := \{1, \dots, \lceil c_1 M^{\kappa} \rceil\}$. Hence, the above construction does provide also an upper bound on the rank parameter in the orthogonal Tucker decomposition, $r \leq C \lceil M^{\kappa} \rceil$, based on *nonlinear approximation* with a fixed tensor-product index set \mathcal{J}^M as the domain for the core tensor.

The rank estimates (2.10) are derived before the discretization in the physical variable $x \in D$. Analogous bounds for fully discrete solutions of the Galerkin system of equations will be addressed in §3 (cf. Proposition 3.3 there).

In the case of exponential decay of the input's fluctuation, i.e. (2.6), the low rank approximation (2.9) exhibits a superalgebraic (though subexponential) convergence rate in terms of the cardinality R of the index sets. The number of terms in (2.9) amounts to $O(e^{\beta_1 M^{\kappa/(\kappa+1)}})$, $\kappa = 1/d_0$, indicating exponential complexity in M for the respective discretizations; note, however, that this is offset by the exponential convergence bound $C \exp(-\beta M^{1/\kappa})$.

The following Proposition indicates that in the case of constant coefficients $a_m(x) = \bar{a}_m$, ($m = 0, 1, \dots, M$) we can achieve the exponential convergence rate in the number of terms. Hence, in the case of variable coefficients, the actual separation rank might be expected as much smaller compared with the (possibly pessimistic) upper bound $R = \#\Sigma_M$ appearing in (2.10). Based on the above conjecture and applying efficient tensor approximation methods,

the number of terms in the separable expansion (2.9) can be reduced so as to remove the “curse of dimensionality”.

In the case of spatially homogeneous coefficients, we denote the associated coefficient function and bilinear form by \bar{a}_M and $\bar{A}_M(\cdot, \cdot)$, respectively.

Proposition 2.6 *Assume that the stochastic coefficients are constant, $a_m(x) = \bar{a}_m$ ($m = 0, 1, \dots, M$). Then the solution of equation (2.1) can be presented by explicit formula*

$$u_M(y, x) = \frac{1}{\bar{a}_0 + \sum_{m=1}^M \bar{a}_m y_m} (-\Delta_x)^{-1} f(x), \quad (2.16)$$

where Δ_x is the Laplace operator on $H_0^1(D)$ in variable $x \in \mathbb{R}^{d_0}$.

Under assumptions 1. - 2. on $a_M(x, y)$ as in §2.2, the multivariate coefficient function in (2.16) allows the following R -term separable approximation

$$G(y) := \frac{1}{\bar{a}_0 + \sum_{m=1}^M \bar{a}_m y_m} \approx \sum_{k=1}^R g_1^k(y_1) \dots g_M^k(y_M), \quad \forall y \in I^M,$$

that converges exponentially in R ,

$$\|G(y) - \sum_{k=1}^R g_1^k(y_1) \dots g_M^k(y_M)\|_{L^\infty(\Gamma)} \leq C e^{-\beta R / \log R}, \quad (2.17)$$

where $\beta > 0$ does not depend on M and R .

Proof. Since assumptions 1. - 2. in §2.2 imply $\bar{a}_M \geq (1 - \gamma)a_{\min} > 0$, we apply the improved sinc-quadrature (see [13], Lemma 4.3, Proposition 2.1) to the function $1/x$, with substitution $x = \bar{a}_0 + \sum_{m=1}^M \bar{a}_m y_m$,

$$1/x = \int_0^\infty e^{-xt} dt \approx \sum_{k=-M}^M c_k e^{-xt_k}, \quad \text{for } x \in [(1 - \gamma)a_{\min}, (1 + \gamma)a_{\min}].$$

Following [13], Lemma 4.3, the coefficients $c_k, t_k > 0$ can be derived from the integral representation

$$1/x = \int_{\mathbb{R}} f_2(\omega) d\omega, \quad f_2(\omega) = \frac{\cosh(\omega)}{1 + e^{-\sinh(\omega)}} e^{-x \log(1 + e^{\sinh(\omega)})}$$

by applying the improved sinc-quadrature in [13], Proposition 2.1. To that end, we set $R_0 = x_{\max}/x_{\min} = \frac{1+\gamma}{1-\gamma}$ (corresponds to the scaling $x \in [1, R_0]$ in [13], Lemma 4.3), and

$$\mathfrak{h} = \log(\pi M)/M, \quad t_k = \log(1 + e^{\sinh(k\mathfrak{h})}), \quad c_k = \mathfrak{h} \frac{\cosh(k\mathfrak{h})}{1 + e^{-\sinh(k\mathfrak{h})}},$$

that ensures the convergence rate as in (2.17) with $R = 2M + 1$. Notice that each term in the quadrature representation has rank 1 since $e^{-xt_k} = e^{-t_k \bar{a}_0} \prod_{m=1}^M e^{-t_k \bar{a}_m y_m}$, which completes the proof. ■

Proposition 2.6 implies that the number of terms R in the above constructed decomposition, that allows to achieve an accuracy $\varepsilon = Ce^{-C_1 M^\kappa}$, $\kappa = 1/d_0$, is equal to $R = O(M^\kappa \log M)$, which follows from the analysis of the equation

$$\frac{R}{\log R} = M^\kappa, \quad M \gg 1.$$

Hence, in this case, we arrive at even better than linear-logarithmic complexity in M (sub-linear complexity for $d_0 \geq 2$).

One can expect that in the case of “smooth” coefficients $a_m(x)$ the situation might be very similar to those described in Proposition 2.6. Moreover, we will show that the operator with constant coefficients $a_m(x) = \bar{a}_m$, is a good candidate for the spectrally close preconditioner.

3 Sparse Tensor-Product Galerkin Discretization

So far, the approximations of the solution u_M were *semidiscrete*, i.e. we assumed that the coefficients $\Phi_\alpha(x) \in V_x$ were available exactly. Now, we consider the numerical approximation of these coefficients from Finite Element spaces in the domain D . The sparse tensor FEM-Galerkin approximation of (2.1) is based on the weak formulation (2.5) in the tensor-product Hilbert space V . A key problem is the possibly high dimension M of the parameter domain Γ .

Our goal is to adapt Galerkin discretization schemes of the parametric, deterministic elliptic problems (2.1) to the low rank tensor-structured matrix formats introduced in §2.4.1.

3.1 Galerkin approximation

We consider the case of tensor-product basis functions $\{\phi_{\mathbf{j}}\}$,

$$\phi_{\mathbf{j}}(y, x) = \phi_{j_0}(x) \prod_{m=1}^M \phi_{j_m}(y_m), \quad \mathbf{j} \in \mathcal{J} = J_0 \times J^M, \quad J := \{1, \dots, n\},$$

where $\{\phi_{j_0}(x)\}$ is chosen as the basis set in the Galerkin subspace $X_{N_0} = (X_{n_0})^{d_0} \in H_0^1(D) = (H_0^1(0, 1))^{d_0}$ of tensor-product piecewise linear functions in variable x . In turn, ϕ_{j_m} are piecewise polynomials in variable $y_m \in I$ ($m = 1, \dots, M$), that span the tensor product space $\mathbb{Y}_M = (Y_n)^M$, where Y_n is either

(A) the set of the univariate Legendre polynomials of degree $n - 1$ in y_m ($m = 1, \dots, M$), or
 (B) Y_n could be the space of piecewise constant basis functions in variable y_m , corresponding to the equidistant grid of size $h = 2/n$ (see §4 for numerics).

To build the Galerkin approximation of the initial boundary value problem (2.5) on the tensor-product Hilbert space

$$V_n := \mathbb{Y}_M \otimes X_{N_0} \subset V = \bigotimes_{m=1}^M L^2(I) \otimes H_0^1(D),$$

we search for the solution in the form $u_M^h = \sum_{\mathbf{j} \in \mathcal{J}} u_{\mathbf{j}} \phi_{\mathbf{j}} \in V_n$, that satisfies

$$A_M(u_M^h, v) = f(v) \quad \forall v \in V_n. \quad (3.1)$$

Lemma 3.1 *The Galerkin equation (3.1) has a unique solution which is quasioptimal*

$$\|u_M - u_M^h\|_V \leq C \inf_{v \in V_n} \|u_M - v\|_V,$$

where the constant $C > 0$ does not depend on M , n and N_0 .

Proof. The bilinear form A_M is coercive (cf. Lemma 2.1) and continuous uniformly in M . Then the result follows by Lax-Milgram lemma. \blacksquare

To derive the Galerkin matrix equation, let us choose some rank-1 test and trial functions in the set $\{\phi_{\mathbf{j}}\}$, $\mathbf{j} \in \mathcal{J}$,

$$u(y, x) = u^{(0)}(x) \prod_{m=1}^M u^{(m)}(y_m), \quad v(y, x) = v^{(0)}(x) \prod_{m=1}^M v^{(m)}(y_m),$$

then the associated bilinear form can be written as follows

$$A_M(u, v) = A_0(u, v) + A_y(u, v)$$

with the separable representations,

$$A_0(u, v) = \left[\sum_{i=1}^{d_0} \left\langle a_0(x) \frac{\partial}{\partial x_i} u^{(0)}(x), \frac{\partial}{\partial x_i} v^{(0)}(x) \right\rangle_{L^2(D)} \right] \prod_{\ell=1}^M \langle u^{(\ell)}(y_\ell), v^{(\ell)}(y_\ell) \rangle_{L^2(I)},$$

$$A_y(u, v) = \sum_{m=1}^M \left[\sum_{i=1}^{d_0} \left\langle a_m(x) \frac{\partial}{\partial x_i} u^{(0)}(x), \frac{\partial}{\partial x_i} v^{(0)}(x) \right\rangle_{L^2(D)} \right] \prod_{\ell=1}^M \langle y_\ell^{\delta_{m\ell}} u^{(\ell)}(y_\ell), v^{(\ell)}(y_\ell) \rangle_{L^2(I)},$$

where $\delta_{m\ell}$ is the Kronecker delta.

With the notation $U = \{u_{\mathbf{j}}\}_{\mathbf{j} \in \mathcal{J}} \in \mathbb{R}^{\mathcal{J}}$ for the coefficient tensor, the Galerkin system of linear algebraic equations now reads

$$\mathbf{A}U \equiv (\mathbf{A}_0 + \sum_{m=1}^M \mathbf{A}_m)U = F \quad U, F \in \mathbb{R}^{\mathcal{J}}, \quad (3.2)$$

with the following tensor-product representation of the stiffness matrix and of the respective right-hand side,

$$\mathbf{A}_m = \bigotimes_{\ell=0}^M A_m^{(\ell)}, \quad F = \bigotimes_{\ell=0}^M F^{(\ell)},$$

where

$$A_m^{(\ell)} \in \mathbb{R}^{n \times n}, \quad F^{(\ell)} \in \mathbb{R}^n \quad \ell = 1, \dots, M, \quad A_m^{(0)} \in \mathbb{R}^{N_0 \times N_0}, \quad F^{(0)} \in \mathbb{R}^{N_0},$$

such that for $m = 0, \dots, M$, we have

$$A_m^{(0)} = \left\{ \sum_{i=1}^{d_0} \left\langle a_m(x) \frac{\partial}{\partial x_i} \phi_{p_0}(x), \frac{\partial}{\partial x_i} \phi_{q_0}(x) \right\rangle_{L^2(D)} \right\}_{p_0, q_0=1}^{N_0}, \quad F^{(0)} = \left\{ \langle f, \phi_{q_0} \rangle_{L^2(D)} \right\}_{q_0=1}^{N_0},$$

and

$$A_m^{(\ell)} = \left\{ \langle y_\ell^{\delta_{m\ell}} \phi_p(y_\ell), \phi_q(y_\ell) \rangle_{L^2(I)} \right\}_{p, q=1}^n, \quad F^{(\ell)} = \left\{ \langle 1, \phi_q(y_\ell) \rangle_{L^2(I)} \right\}_{q=1}^n, \quad \ell = 1, \dots, M.$$

The next lemma characterizes the tensor-structured representation of the matrix \mathbf{A} and loading vector F in (3.2).

Lemma 3.2 We have $\mathbf{A} \in \mathcal{M}_{M+1, \mathbf{n}}$ and $F \in \mathcal{C}_{1, \mathbf{n}}$ with $\mathbf{n} = (N_0, n, \dots, n)$. The storage requirements to represent the matrix \mathbf{A} and the rank-1 vector F are estimated by

$$Q(\mathbf{A}) = O(N_0M + n^\alpha M), \quad \alpha = 1, 2, \quad Q(F) = O(N_0 + nM),$$

respectively. Here $\alpha = 1$ corresponds to the piecewise constant elements, and $\alpha = 2$ appears in the case of Legendre polynomials. The matrix-times-vector multiplication of \mathbf{A} with an rank-1 tensor in $\mathcal{C}_{1, \mathbf{n}}$, scales linearly in M , $O(N_0M + nM)$.

Proof.

The storage for sparse FEM stiffness matrices $A_m^{(0)}$, ($m = 0, \dots, M$), is estimated by $O(N_0M)$. Depending on the choice of basis functions in \mathbb{Y}_M , the sparsity of matrices $A_m^{(\ell)}$ ($\ell = 1, \dots, M$, $m = 1, \dots, M$) is characterized by the value n^α , $\alpha = 1, 2$, where the set of matrices $A_m^{(\ell)}$, ($1 < m \leq M$), is obtained by cyclic repetition of $A_1^{(\ell)}$. Considerations for the loading vector F are similar.

Suppose now that the vector $U \in \mathbb{R}^{\mathcal{J}}$ has rank-1 tensor representation (see Appendix)

$$U = u^{(0)} \otimes \dots \otimes u^{(M)}, \quad u^{(\ell)} \in \mathbb{R}^n, \quad \ell = 1, \dots, M; \quad u^{(0)} \in \mathbb{R}^{N_0}.$$

Then the matrix-times-vector multiplication with \mathbf{A} is reduced to the univariate algebraic operations,

$$\mathbf{A}U = \sum_{m=0}^M \bigotimes_{\ell=0}^M A_m^{(\ell)} u^{(\ell)},$$

that proves the second assertion, taking into account the repeating terms in the respective tensor products. \blacksquare

We complete §3.1 by an illustration on the tensor structure of the stiffness matrix \mathbf{A} .

Example 1. Let $d_0 = 1$, $M = 2$, and let Y_n be the space of piecewise constant basis functions over the uniform grid of size n in each variable y_m , $m = 1, 2$. Then $A_m^{(0)} \in \mathbb{R}^{n_0 \times n_0}$, $m = 0, 1, 2$ are symmetric, positive definite and tridiagonal matrices. The mass matrices in variable y_m are diagonal ones. Denoting $A_1^{(1)} = A_2^{(2)} = Z \in \mathbb{R}^{n \times n}$, and $A_m^{(\ell)} = W = hI_n \in \mathbb{R}^{n \times n}$ (scaled identity), otherwise, the resultant rank-3 stiffness matrix takes the form

$$\mathbf{A} = W \otimes W \otimes A_0^{(0)} + Z \otimes W \otimes A_1^{(0)} + W \otimes Z \otimes A_2^{(0)}.$$

To construct the preconditioner, this matrix can be first factorized as

$$\mathbf{A} = (W \otimes W \otimes A_0^{(0)})B,$$

with

$$B = I_n \otimes I_n \otimes I_{n_0} + W^{-1}Z \otimes I_n \otimes (A_0^{(0)})^{-1}A_1^{(0)} + I_n \otimes W^{-1}Z \otimes (A_0^{(0)})^{-1}A_2^{(0)},$$

where $W^{-1}Z$ is spectrally equivalent to I_n uniformly in n , while both the matrix $(A_0^{(0)})^{-1}A_1^{(0)}$, and $(A_0^{(0)})^{-1}A_2^{(0)}$, are spectrally equivalent to I_{n_0} . Preconditioning matrix is then given by $W^{-1} \otimes W^{-1} \otimes A_0^{(0)-1}$.

3.2 Canonical and Tucker rank estimates

Application of tensor formats for solution of large linear system of equations (3.2) requires the low tensor rank representations of all matrices and vectors arising in the computational process.

The rank estimates for the solutions of the discrete Galerkin equation can be derived from [4]. Let the index set $\Sigma_{M,\mu,\nu} \subset \mathcal{J}^M \subset \mathbb{N}_0^M$ be defined by

$$\Sigma_{M,\mu,\nu} := \{\alpha \in \mathcal{J}^M : |\alpha|_0 \leq \nu, |\alpha|_1 \leq \mu\}.$$

Introducing the respective approximation

$$u_{\Sigma_{M,\mu,\nu}}^h = \sum_{\alpha \in \Sigma_{M,\mu,\nu}} u_\alpha y^\alpha, \quad u_\alpha \in X_{N_0},$$

as in [4, Proposition 3.11], the relation between the approximation error and the cardinality bound can be derived as follows.

Proposition 3.3 *There exist constants $C_M, c_\mu, c_\nu > 0$, independent of M, μ, ν , such that for any $\varepsilon > 0$, by choosing $h = O(\varepsilon)$,*

$$M = \lceil c_M |\log \varepsilon|^{d_0} \rceil, \quad \mu = \lceil c_\mu M^\kappa \rceil, \quad \nu := \lceil c_\nu M^{\kappa/\kappa+1} \rceil, \quad \kappa = 1/d_0,$$

we have

$$\|u_M - u_{\Sigma_{M,\mu,\nu}}^h\|_{V_x} \leq \varepsilon, \quad \forall y \in \Gamma,$$

and for any fixed $s > 0$, as $\varepsilon \rightarrow 0$, we have the bound

$$\#\Sigma_{M,\mu,\nu} \leq C\varepsilon^{-1/s}.$$

The rank estimates for the solution of the discrete Galerkin equation (3.2) is a consequence of Proposition 3.3.

Lemma 3.4 *For given $\varepsilon > 0$, and for any fixed $s > 0$, the solution u_M with parameters M, μ, ν , chosen as above, has the canonical and Tucker ranks at most*

$$R = O(\varepsilon^{-1/s}), \quad \text{and} \quad r = O(\max\{M^{1/d_0}, N_0\}),$$

respectively. There is the sparse Tucker approximation with the number of nonzero terms not exceeding $C\varepsilon^{-1/s}$.

Proof. Choose the approximation $u_{\Sigma_{M,\mu,\nu}}^h$ of u_M with parameters M, μ, ν , as in Proposition 3.3 and take into account that $\Lambda_{M,\mu,\nu} \subset \mathcal{J}^M$ holds. Then the first assertion follows directly from definitions of the canonical and Tucker ranks as in Appendix. To prove the second statement, we note that the approximand $u_{\Lambda_{M,\mu,\nu}}^h$ is just the Tucker sum over index set $\mathcal{J}^M \times \mathbb{R}^{N_0}$, with the number of nonzero terms bounded by $\#\Lambda_{M,\mu,\nu}$. This completes our proof. \blacksquare

There is still an open question either some better estimates on the canonical and Tucker ranks of the respective nonlinear approximations are possible (cf. Proposition 2.6). Finding the rigorous answer on this question, first, requires the extensive numerical study.

3.3 Analysis of low tensor rank preconditioners

For the robust and fast convergence of the iterative solvers for high-dimensional equation (3.2), we need the simple spectrally close preconditioners that can be also represented in the low tensor rank format (see Appendix). In this section we describe two classes of low rank preconditioners.

Introduce the bilinear form \bar{A}_M on the tensor-product Hilbert space V ,

$$\bar{A}_M(u, v) := \int_{\Gamma} \int_D \bar{a}_M(y, x) \nabla_x u \cdot \nabla_x v dx dy, \quad u, v \in V,$$

where the coefficient is given by constants \bar{a}_m ($m = 0, 1, \dots, M$) as follows

$$\bar{a}_M(y, x) := \bar{a}_0 + \sum_{m=1}^M \bar{a}_m y_m.$$

Next statement gives the spectral equivalence estimates for preconditioners generated by the bilinear forms A_0 and \bar{A}_M .

Lemma 3.5 *The spectral equivalence*

$$(1 - \gamma) \langle \mathbf{A}_0 U, U \rangle_{V_n} \leq \langle \mathbf{A} U, U \rangle_{V_n} \leq (1 + \gamma) \langle \mathbf{A}_0 U, U \rangle_{V_n} \quad \forall U \in V_n, \quad (3.3)$$

holds uniformly in N_0 and n . Moreover, assume that the operator coefficient $a_m(x)$, is a "small" perturbation of its meanvalue $\bar{a}_m \geq 0$ over D ,

$$|a_m(x) - \bar{a}_m| \leq \alpha \bar{a}_m, \quad m = 0, \dots, M, \quad (3.4)$$

with some $1 > \beta > 0$, such that $\gamma \leq \frac{1}{1-\beta}$, and $\frac{1}{1-\beta} + \gamma < \frac{1-\gamma}{\beta}$. Then the bilinear form \bar{A}_M generates the spectrally equivalent preconditioner $\bar{\mathbf{A}}_M$ to \mathbf{A} , characterized by the equivalence constants $C_0 = \left[1 + \frac{\beta}{1+\gamma} \left(\frac{1}{1-\beta} - \gamma\right)\right]^{-1}$, and $C_1 = \left[1 - \frac{\beta}{1-\gamma} \left(\frac{1}{1-\beta} + \gamma\right)\right]^{-1}$.

Proof. Using conditions 1) - 2) (cf. §2.2) and the strong ellipticity criteria (2.3), the first spectral equivalence estimate then follows from the two-sided bound

$$(1 - \gamma)A_0(u, u) \leq A_M(u, u) \leq (1 + \gamma)A_0(u, u) \quad \forall u \in V,$$

to be considered on the Galerkin subspace $V_n \subset V$.

The second assertion is obtained by estimating $a_M(y, x)$ by means of the respective coefficient expansion,

$$a_M(y, x) := \bar{a}_M(y, x) + a_0(x) - \bar{a}_0 + \sum_{m=1}^M (a_m(x) - \bar{a}_m) y_m,$$

and taking into account (3.4),

$$\bar{a}_M(y, x) - \beta(1/(1 - \beta) - \gamma)a_0(x) \leq a_M(y, x) \leq \bar{a}_M(y, x) + \beta(1/(1 - \beta) + \gamma)a_0(x).$$

Based on (3.3), the latter inequalities imply,

$$\left[1 + \frac{\beta}{1+\gamma} \left(\frac{1}{1-\beta} - \gamma\right)\right]^{-1} \overline{\mathbf{A}}_M \leq \mathbf{A} \leq \left[1 - \frac{\beta}{1-\gamma} \left(\frac{1}{1-\beta} + \gamma\right)\right]^{-1} \overline{\mathbf{A}}_M,$$

which completes the proof. \blacksquare

The previous lemma ensures that one class of efficient preconditioners is generated by the bilinear form A_0 , i.e., it is defined by any low rank approximation to the matrix \mathbf{A}_0^{-1} . Detailed discussion on such kind of approximation can be found in [20].

The second class is based on the averaging approximation with constant coefficients \bar{a}_m , $m = 1, \dots, M$. In this case, the low rank representation to $\overline{\mathbf{A}}_M^{-1}$ is described in Proposition 2.6.

3.4 Tensor-structured iteration with rank truncation

Lemmata 3.2 and 3.5 provide the starting point to design the fast tensor methods of almost linear complexity in both N_0 and n , and with exponential scaling like r^M ($r = O(|\log \varepsilon|)$) when using the Tucker format. In the case of rank- R solution u_M , we can expect even the linear-logarithmic scaling $O(MR(N_0 + n))$.

To fix the point, consider the system of *linear* algebraic equations

$$U \in \mathcal{S} \subset \mathbb{R}^{\mathcal{J}} : \quad \mathbf{A}U = F, \quad F \in \mathcal{C}_1, \quad (3.5)$$

posed on certain *nonlinear manifold* \mathcal{S} of rank-structured tensors. We apply the simple *preconditioned Jacobi iteration* accomplished with the *rank optimization* procedure at each iterative step. To that end, let us introduce the *truncation operator* $T_R : \mathbb{R}^{\mathcal{J}} \rightarrow \mathcal{S}$, which is the nonlinear operator that defines the best rank-structured approximation in the form

$$A \in \mathbb{R}^{\mathcal{J}} : \quad T_R(A) := \operatorname{argmin}_{X \in \mathcal{S}} \|X - A\|. \quad (3.6)$$

The truncation operator in (3.6) can be defined on different classes of rank structured tensors, say, on the Tucker or two-level Tucker formats [18]. Furthermore, the recently analysed dimension splitting TC/TT tensor formats can be considered [30, 28, 22].

Several heuristic methods for computing the corresponding rank structured approximations in different classes of input/output tensors were discussed in the literature [7, 26, 36, 23, 29, 18]. It is worth to note that the orthogonal Tucker approximation as well as approximations in the dimension splitting tensor formats [28, 31, 11, 22] can be realized by using QR/SVD-based schemes with the quasioptimal error bound. We also stress that using the recently introduced *quantics-type approximation* of tensors (cf. [22]) it might be possible to achieve the log-scaling of the numerical algorithm in both the volume size and the approximation error, $O(M \log n \log \varepsilon^{-1})$.

Based on the results in [22, Proposition 3.5], [31], [8, 23], next statement shows that the tensor truncation operator $T_{\mathcal{S}}$, associated with the Tucker and TC-formats, provides the quasioptimal SVD-based approximation on the tensor manifold with fixed rank parameters.

Proposition 3.6 (*Tensor truncation*). *The operator $T_{\mathcal{S}} : \mathbb{V}_{\mathbf{n},d} \rightarrow \mathcal{S} := TC[\mathbf{r}, \mathbf{n}, d]$ is well defined. The same holds true for the Tucker truncation operator.*

For given $A_0 \in TT[\mathbf{r}_0, \mathbf{n}, d] \subset \mathbb{V}_{\mathbf{n}, d}$, and $\mathbf{r} < \mathbf{r}_0$, the quasioptimal approximation to $T_{\mathcal{S}}A_0$ can be computed by finite QR/SVD based algorithm in $O(ndr_0^3)$ operations. The Tucker truncation can be computed by the ALS iteration provided that the initial guess is given by the higher order SVD (cf. [8]).

If $A_0 \in \mathcal{C}_R$, then the quasioptimal rank- r Tucker approximation can be computed by SVD-based RHOSVD algorithm (cf. [23]).

In our numerical experiments we test the tensor truncation to the set of rank- R canonical tensors, $\mathcal{S} = \mathcal{C}_R$. Respectively, we denote $T_{\mathcal{S}} = T_R$. In this case, the only approximate solution of the problem (3.6) can be (iteratively) computed. In the current implementation, we apply the heuristic *multistep enhanced ALS iteration* to perform the rank optimisation in the canonical format [21].

To proceed with, we introduce the tensor-truncated iteration as follows. Given $U^{(0)} \in \mathcal{C}_R$, calculate for $m = 1, 2, \dots$ till termination:

$$\tilde{U}^{(m+1)} := U^{(m)} - \omega \mathbf{B} (\mathbf{A}U^{(m)} - F), \quad U^{(m+1)} = T_R(\tilde{U}^{(m+1)}) \rightarrow U, \quad (3.7)$$

with some $\omega > 0$, where \mathbf{B} can be chosen as one of the low tensor rank preconditioners introduced above, $\mathbf{B} = \mathbf{A}_0^{-1}$ or $\mathbf{B} = \overline{\mathbf{A}}_M^{-1}$.

For example, with the choice $\mathbf{B} = \mathbf{A}_0^{-1}$, $\omega = 1$, $T_R = I$, the spectral bounds $sp(\mathbf{A}_0^{-1}\mathbf{A}) \in [1 - \gamma, 1 + \gamma]$ can be proved (see Lemma 3.5), and we obtain in (3.7) the exact fixed point iteration with the contraction factor $q = \gamma < 1$. Hence, if the truncation operator is accurate enough, that can be achieved by increasing the truncation rank in the intermediate iterative steps to some $R' > R$, the contraction factor in (3.7) can be controlled by some $q' < 1$.

In the (nonlinear) iteration (3.7) the truncation operator T_R can be applied to the residual vectors $\mathbf{A}U^{(m)} - F$, and $\mathbf{B}(\mathbf{A}U^{(m)} - F)$, as well.

Notice that the target tensor $X \in \mathbb{R}^{\mathcal{J}}$ in (3.6) can be approximated by a sum of rank-1 tensors as in (2.12), and (2.13). In the case $M = 1$, i.e. for $d = 2$, these two representations are equivalent, and they can be computed by the so-called ‘‘truncated’’ SVD. In the general case of $M \geq 2$, the action of truncation operator is reduced to the nonlinear approximation problem in the corresponding multilinear algebra setting as in (3.6).

4 Numerical illustrations

4.1 Performance of the low tensor rank preconditioners

Consider the case of spatially homogeneous stochastic coefficients,

$$a(y, x) = a(y) := 1 + \sum_{m=1}^M a_m y_m \quad \text{with} \quad \gamma = \|\mathbf{a}\|_{\ell_1} := \sum_{m=1}^M |a_m| < 1, \quad (4.1)$$

for the truncated sequence of (spatially homogeneous) coefficients $a_m = (1 + m)^{-\alpha}$, ($m = 1, \dots, M$) with algebraic decay rates $\alpha = 2, 3, 5$ (In this section the parameter α corresponds to the decay rate parameter s introduced in §2.3). We compute the rank- R tensor approximation to the preconditioning matrix $\overline{\mathbf{A}}_M^{-1}$, corresponding to the multivariate function $a(y)^{-1}$

over the tensor-product grid of size $n^{\otimes M}$. For different values of the rank parameter R , dimension parameter $M = 10, 20, 50, 100$, and for the univariate grid size $n = 2^p$, $p = 6$, we use the rank- R approximation based on the sinc-quadratures, as in Proposition 2.6, where $R = 2L + 1$.

We present the results for y -dependent factor in the rank- R approximation to the inverse matrix $\overline{\mathbf{A}}_M^{-1}$ (see Lemma 3.5 and Proposition 2.6) tested on the rank-1 random vector of size $n^{\otimes M}$. The approximation error is measured at fixed sampling points of the M -fold tensor product space \mathbb{Y}_n^M . The results are depicted in Figures 4.1, 4.2, 4.3, and 4.4.

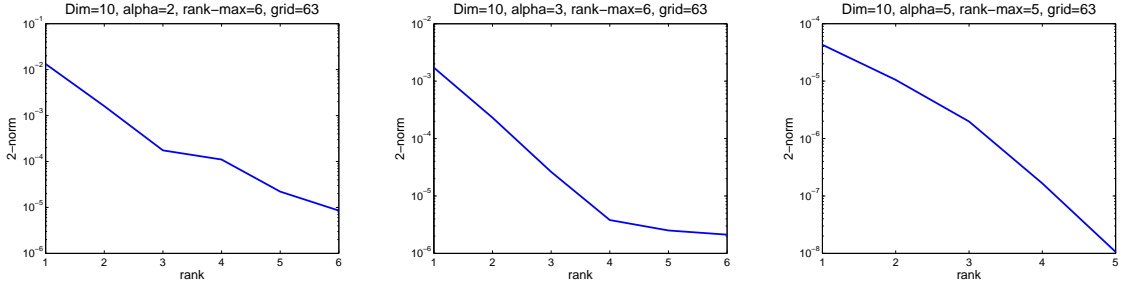


Figure 4.1: Approximation error vs. rank R for $\overline{\mathbf{A}}_M^{-1}$ with $M = 10$, $a_m = a_m(\alpha)$.

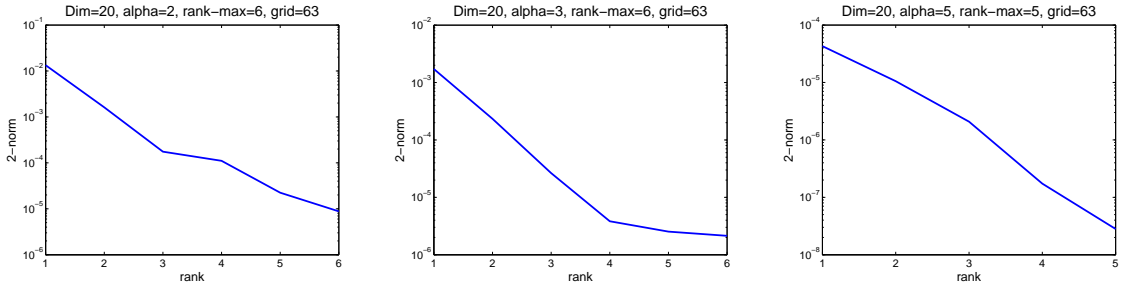


Figure 4.2: Approximation error vs. rank R for $\overline{\mathbf{A}}_M^{-1}$ with $M = 20$, $a_m = a_m(\alpha)$.

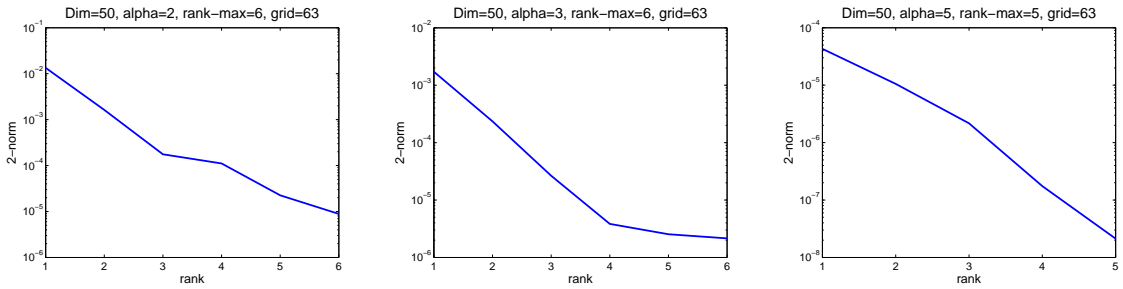


Figure 4.3: Approximation error vs. rank R for $\overline{\mathbf{A}}_M^{-1}$ with $M = 50$, $a_m = a_m(\alpha)$.

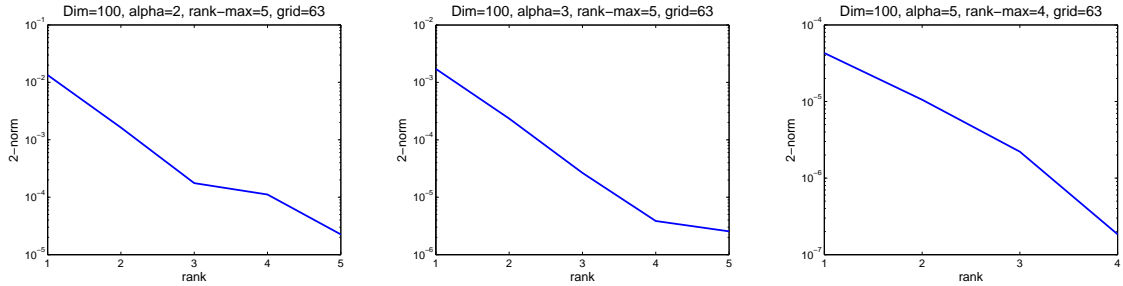


Figure 4.4: Approximation error vs. rank R for $\overline{\mathbf{A}}_M^{-1}$ with $M = 100$.

We observe fast exponential convergence of the rank- R approximation even in the case of slow, algebraic decay of the expansion coefficients (e.g. for $\alpha = 2$). Another important observation is that the convergence rate with respect to R is uniform in the stochastic dimension, at least in the range $10 \leq M \leq 100$.

4.2 Preconditioning: spatially homogeneous random coefficients

In the next example, we apply the truncated iteration (3.7) with the rank-1 preconditioner $\mathbf{B} = \mathbf{A}_0^{-1}$ for solving the discrete sPDE with the constant stochastic coefficient $a_m(x) = \text{const}$ ($m = 1, \dots, M$) as in (4.1) and with given right-hand side $f = 1$. Since in the case $a_m(x) = \text{const}$, we are able to calculate the exact solution with any prescribed accuracy, we present the results on the approximation error vs. the rank parameter for the rank structured solutions of the equation (3.5). We consider the case $d_0 = 1$ for the physical dimension, and discretise the elliptic part by piecewise linear finite elements with same grid size as for the stochastic variables.

The results on low tensor-rank approximation of the exact solution U , calculated for different dimension parameters $M = 10, 20, 50$, and grid size $n = 31, 63$, are presented in Figures 4.5, 4.6, and 4.7.

The convergence history for the rank-structured truncated iteration for solving the system of linear equations (3.5) in the total dimension $d = M + 1$, with $M = 20, 30, 40$, and $a_m = a_m(\alpha)$, is depicted in Figure 4.8. Here T-iter means the number of truncated iterations, performed for different values of the truncation rank parameter R .

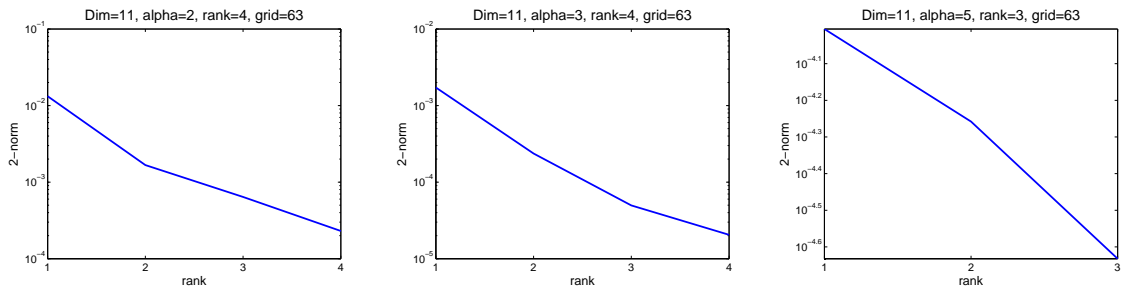


Figure 4.5: Low rank approximation for solutions of sPDE with $M = 10$, and $a_m(x) = \text{const}$.

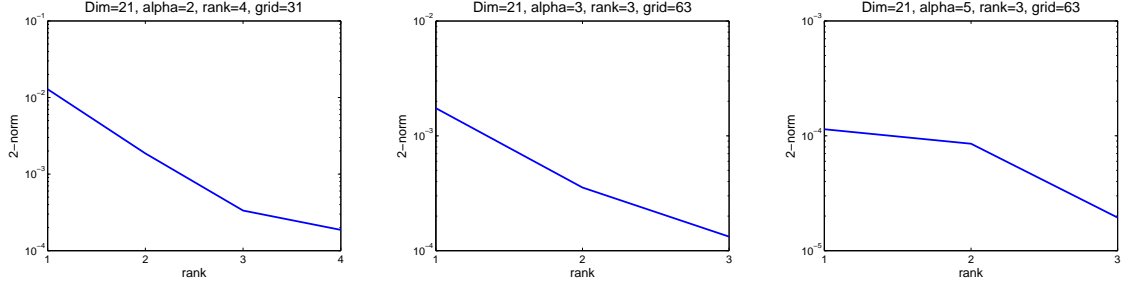


Figure 4.6: Low rank approximation for solutions of sPDE with $M = 20$, and $a_m(x) = \text{const.}$

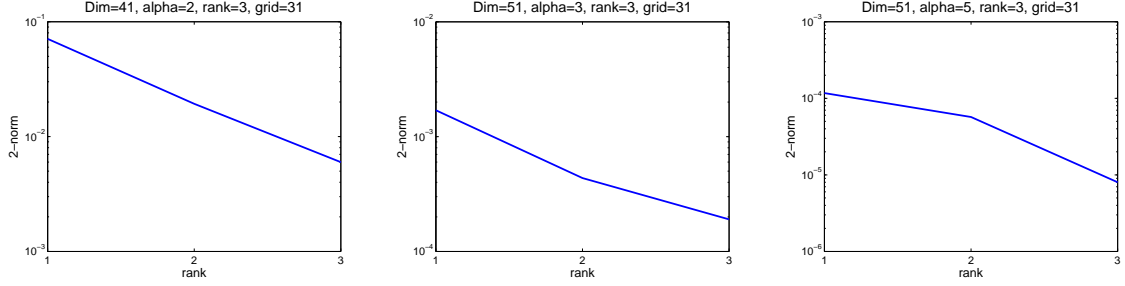


Figure 4.7: Low rank approximation for solutions of sPDE with $M = 40, 50$, and $a_m(x) = \text{const.}$

4.3 Preconditioned iteration: variable stochastic coefficients

In the following example, we apply the truncated iteration (3.7) with the rank-1 preconditioner \mathbf{A}_0^{-1} to the equation (2.1) with variable coefficients (polynomial decay)

$$a_m(x) = (1 + m)^{-\alpha} \sin(mx), \quad m = 1, 2, \dots, M, \quad x \in (0, \pi),$$

and with $a_0 = 1$. The right-hand side in (2.1) is given by $f(x) = \sin(x)$. We present the convergence history for the dimension parameter $M = 20$, and fixed grid-size $n = 31$, in all variables $x \in (0, \pi)$, and $y_m \in (-1, 1)$. Again, we use piecewise linear finite elements

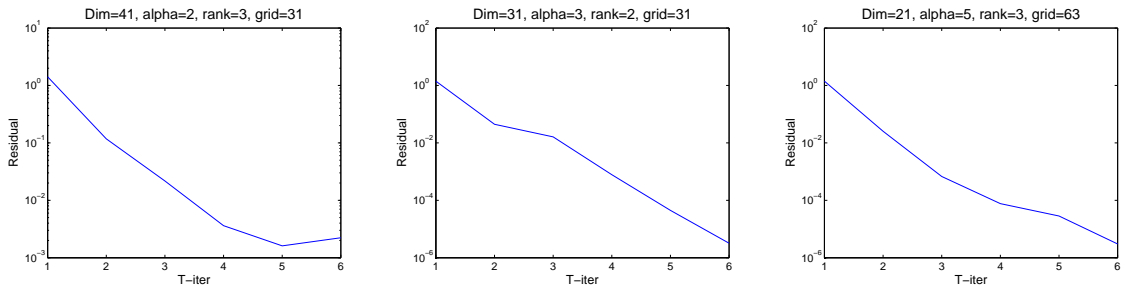


Figure 4.8: Convergence history for truncated preconditioned iteration to solve sPDE with $M = 20, 30, 40$, and $a_m(x) = \text{const.}$

in x and piecewise constant approximation in the stochastic variables y_m . We also vary the parameter $\alpha = 2, 3, 4$ and the truncation rank $R = 1, 2, 3$. Figure 4.9 represents the approximation error vs. rank parameter, while Figure 4.10 gives the convergence history vs. the number of truncated iterations.

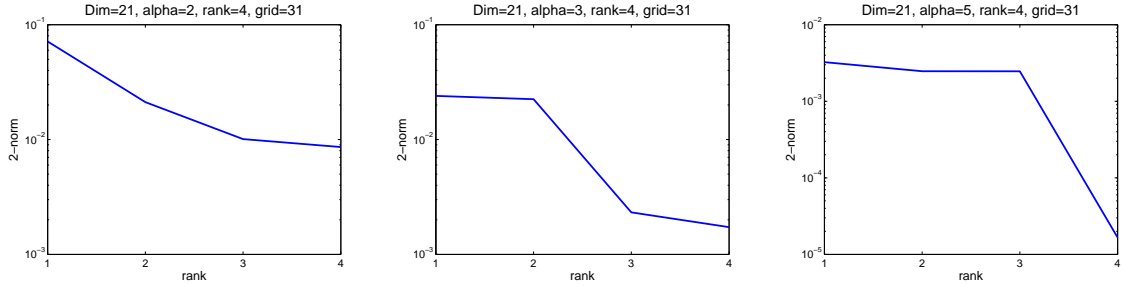


Figure 4.9: Low rank approximation for solutions of sPDE with $M = 20$, and $a_m(x) = c_m(\alpha) \sin(mx)$ (polynomial decay).

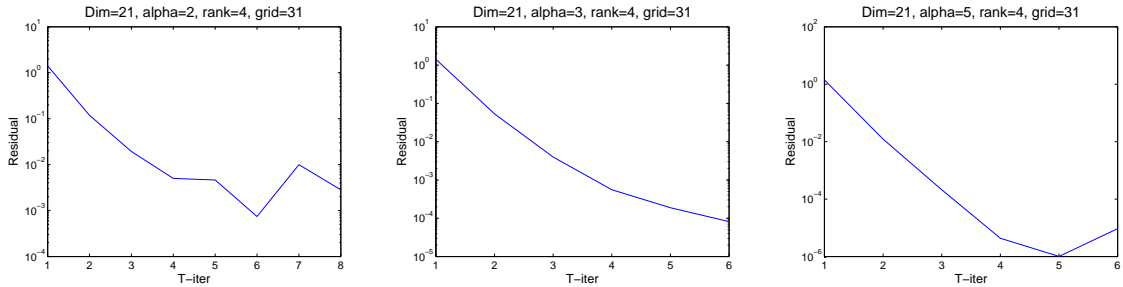


Figure 4.10: Convergence history for tensor truncated iteration to solve the sPDE with $M = 20$, and $a_m(x) = c_m(\alpha) \sin(mx)$ (polynomial decay).

In the last numerical example, we consider variable coefficients with exponential decay,

$$a_m(x) = 0.5 e^{-\alpha m} \sin(mx), \quad m = 1, 2, \dots, M, \quad x \in (0, \pi).$$

The results for $\alpha = 1, 2$, $n = 63$, $R = 5$, are depicted in Figures 4.11, 4.12 and 4.13. In particular, examples of canonical vectors for rank- R solutions of sPDE are given in Figure 4.13.

5 Conclusions

In the present paper we proposed a new class of low-rank tensor based numerical methods for solving PDEs with random inputs. We presented theoretical and numerical evidence that our method scales linearly in the dimension M of stochastic input parameter space.

Our approach is based on low rank separable representation to the discrete multivariate functions and operators (matrices) involved in the FEM-Galerkin approximation.

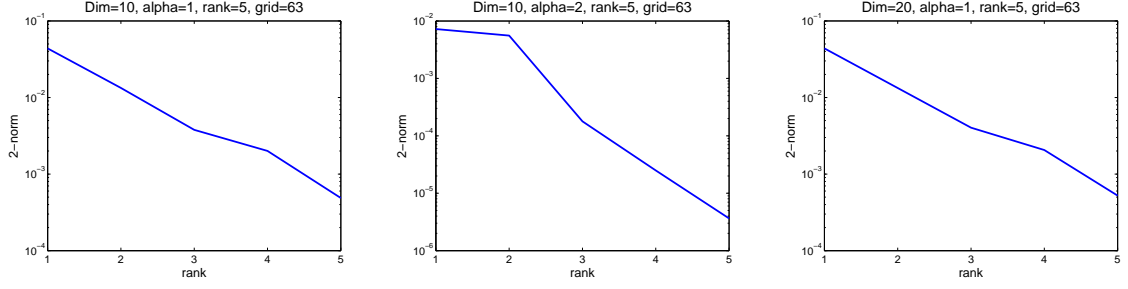


Figure 4.11: Low rank approximation for solutions of sPDE with $M = 10, 20$ and $a_m(x) = e^{-\alpha m} \sin(mx)$ (exponential decay).

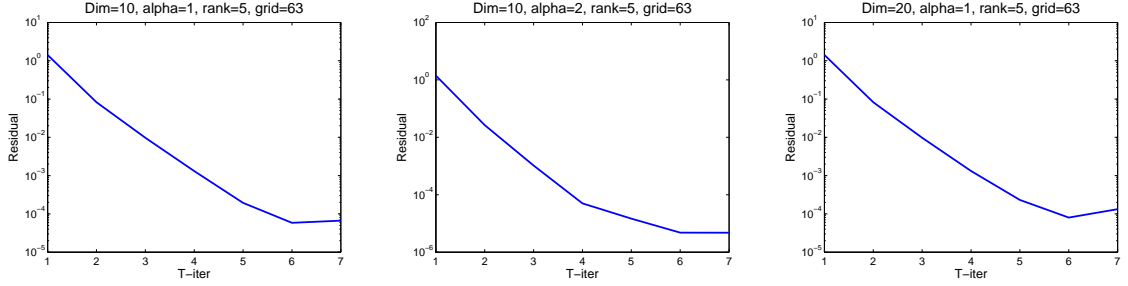


Figure 4.12: Iteration history for solutions of sPDE with $M = 10, 20$ and $a_m(x) = e^{-\alpha m} \sin(mx)$ (exponential decay).

Preliminary conclusions based on the numerical experiments in the present paper are the following:

1. The solutions of parametric sPDEs can be well represented with low separation rank.
2. The preconditioned truncated iteration demonstrates the monotone and robust geometric convergence (as expected).
3. The convergence of rank-reduced formatted tensor approximations is faster for larger values of α , i.e., for faster decay of the stochastic coefficients (as expected).
4. For the fixed error bound $\varepsilon_0 > 0$, the dimensionality parameter M should be related to the decay rate α by the equations $(1 + M)^{-\alpha} \approx \varepsilon_0$, or $e^{-\alpha M} \approx \varepsilon_0$ (as expected).
5. For larger dimension M , the approximation ranks determined by the proposed algorithms remain uniformly bounded independently of M .
6. Computational time and storage requirements scale linearly in the univariate grid-size n and nearly linearly in M . Therefore, solutions of parametric deterministic PDEs with smooth dependence on the parameters resulting from random input parameters can be solved at least for a moderately large number M of input parameters (in the present work, $M \leq 50$).
7. Low rank approximations converge faster in the case of exponential decay of coefficients a_m compared to the case of polynomial decay.
8. There are still many open questions, hence further theoretical and algorithmic developments are required. In particular, applications of the more flexible rank-decompositions than the canonical tensor format can be addressed in the future works.

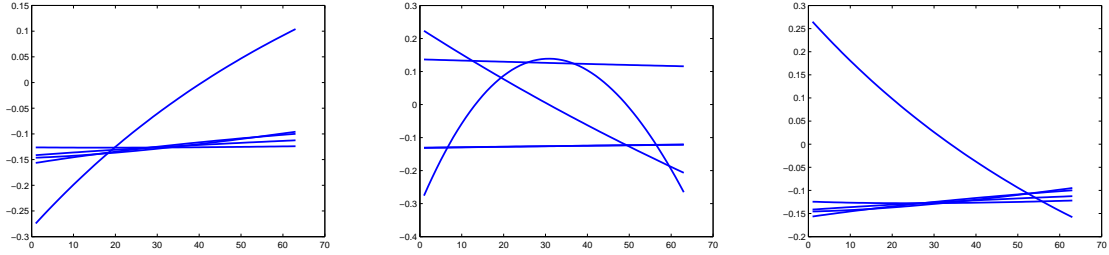


Figure 4.13: First of ℓ -mode canonical vectors ($\ell = 1, 2, 3$) for solutions of sPDE with $d_0 = 1$, $M = 10, 20$ and spatially inhomogeneous random coefficients $a_m(x) = e^{-\alpha m} \sin(mx)$ (exponential decay).

9. The preliminary conclusion from the present work is that low-rank structured tensor approximations of the solution of parametric deterministic PDEs on high dimensional parameter spaces seems to be a promising concept. It allows for the efficient, matrix based numerical solution of discretized deterministic PDEs on high dimensional parameter spaces with linear scaling complexity on the dimension of the parameter space.

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