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# QUANTICS-TT COLLOCATION APPROXIMATION OF PARAMETER-DEPENDENT AND STOCHASTIC ELLIPTIC PDES

B.N. KHOROMSKIJ [1] AND I. OSELEDETS[2]

**Abstract** — We investigate the convergence rate of the quantics-TT (QTT) stochastic collocation tensor approximations to solutions of multiparametric elliptic PDEs and construct efficient iterative methods for solving arising high-dimensional parameter-dependent algebraic systems of equations. 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. We consider both the case of additive and log-additive dependence on the multivariate parameter. The local-global versions of the QTT-rank estimates for the system matrix in terms of the parameter space dimension is proven. Similar rank bounds are observed in numerics for the solutions of the discrete linear system. We propose QTT-truncated iteration based on the construction of solution-adaptive preconditioner that provides robust convergence in both additive and log-additive cases. Various numerical tests indicate that the numerical complexity scales almost linearly in the dimension of parametric space $M$.

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## 1. Introduction

In recent years, tensor-structured numerical methods based on the separation of variables have proved their value in multidimensional problems of computational chemistry [4, 29, 7, 14, 13], quantum molecular dynamics [21, 19], quantum computation [28], and stochastic PDEs [27, 26, 5, 10, 20, 16]. In particular, low-rank tensor approximations in canonical format for stochastic PDEs were recently introduced in [16] (see also [18]).

In the present paper, we investigate the convergence rate of the quantics-TT (QTT) stochastic collocation tensor approximations for solving deterministic parametric elliptic equations in a high dimensional parameter space, arising, for example, as a projection of the stochastic PDE via a *truncated $M$-term Karhunen-Loève expansion.* In general, the model problem has the form

$$\mathcal{A}(y)u = f \quad \text{in } D \in \mathbb{R}^{d_0}, \tag{1.1}$$

$d_0 = 1, 2, 3$, where $\mathcal{A}(y)$ is an elliptic operator in a domain $D$, with a coefficient depending on a certain multidimensional parameter $y \in \mathbb{R}^M$, where $M$ can vary from several tens to several hundreds. In the case of stochastic PDEs, we consider a class of model elliptic

[1] *Max-Planck-Institut für Mathematik in den Naturwissenschaften,* Inselstr. 22-26, D-04103 Leipzig, Germany. E-mail: bokh@mis.mpg.de

[2] *INM RAS,* Gubkina str. 8, Moscow, Russia. E-mail: ivan@bach.inm.ras.ru

problems characterized by the additive/log-additive dependence of the equation coefficients on the multivariate parameter $y$, corresponding to a random field that is linear/exponential in the random variable. Stochastic Galerkin approximations of equations (1.1) via sparse finite elements were introduced in [2, 26], and the stochastic-collocation method for elliptic PDEs was described in detail in [1].

The QTT representation gives log-volume complexity in the number of elements of the tensor for several important problems [23, 12, 15]. For both the additive and the log-additive cases, we prove local and global versions of QTT-rank estimates for the system matrix in terms of the parameter space dimension. We show that in some cases faster numerical algorithms can be designed using the localised version of QTT and canonical formats (cf. [13]). In particular, the local-QTT rank of the system matrix is proven to be uniformly bounded in $M$, while its global rank is shown by numerical experiments to increase at most linearly in $M$. Uniform QTT rank bounds are observed in numerical tests for the solutions of respective discrete linear systems.

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 tensors represented in QTT format. The numerical cost of the matrix-vector multiplication in our setting scales linear in $M$, and in the discrete (physical) problem size $N$.

To enhance the convergence of the global solver, we propose the preconditioned block Jacobi-type iteration accomplished with rank optimization at each iterative step. Our basic rank-1 preconditioner is constructed using the tensor-product approximation to the parametric elliptic operator inverse with spatially homogeneous random coefficients. The overall numerical cost is estimated by $O(M^3 \log N) - O(M^4 \log N)$ provided that the QTT rank of the system matrix is bounded by $O(M)$.

The rest of the paper is organized as follows. In §2, we set up the problem in the case of additive and log-additive coefficient dependence on the multivariate parameter. In §3, we first present the definitions of tensor structured vector- and matrix-formats to be utilized in the paper. We then discuss the tensor-product FEM-collocation scheme and prove the rank bounds for the resulting system matrix. We describe the basic low tensor rank preconditioner, prove its spectral equivalence, and introduce the respective iterative solvers with adaptive rank optimization via the QTT nonlinear approximation. In §4, we give various numerical examples corresponding to stochastic PDEs with variable stochastic coefficients in the case of random fields that are linear/exponential in the random variable. We investigate the case of both polynomial and exponential decay of stochastic coefficients. Numerical examples for elliptic equations with jumping parameter-dependent coefficients are also presented.

## 2. Parameter-Dependent Elliptic Problem

### 2.1. Weak formulations and solvability

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 domain $\Gamma := (-1,1)^M \equiv I^M$, $M \in \mathbb{N}$. We are given $f \in L^2(D)$, and a parametric elliptic operator

$$\mathcal{A}(y) := -\mathrm{div}_x \left(a(y,x)\mathrm{grad}_x\right), \quad y \in \Gamma,$$

where the coefficient $a(y,x) = a_M(y,x)$ is a smooth function of $x \in D$ and the parameter vector $y = (y_1, ..., y_M) \in \Gamma$ with a possibly very large number $M$ of parameters. We formulate

the problems in the tensor-product Hilbert space (cf. [16]),

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

Specifically, 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

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

In this problem setting the dimension $M$ of the parametric space corresponds to the truncation parameter in the Karhunen-Loève expansion. In discretization of diffusion problems with random inputs, the dimension $M$ of the parameter space could become arbitrarily large.

We consider the class of problems, with the *additive and log-additive* dependence of the coefficient function on $y \in \Gamma$.

In the *additive case*, the coefficient function is defined by

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

with $a_m \in L^\infty(D)$, $m = 1, ..., M$. Concerning the coefficient function $a_M(y,x)$, we assume (see [16]) that there exists $a_{min} > 0$, such that

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

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

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

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 in accordance with (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 $y \in \Gamma$. Under assumptions 1) - 2), we have a 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

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

In elliptic problems, the coefficient $a(x,y)$ should be positive, which is not automatically satisfied by the affine mode (2.2), and it would be more natural to have the operator coefficient $a$ in the form (the so-called *log-additive case*),

$$a(y,x) = e^{a_M(y,x)} = e^{a_0(x)} \prod_{m=1}^{M} e^{a_m(x) y_m}.$$

Conditions 1) - 2) imply spectral equivalence relations in the physical variables,

$$C_0\langle A_0 u, u\rangle \leqslant \langle Au, u\rangle \leqslant C_1\langle A_0 u, u\rangle, \quad \forall\, u \in V_x, \tag{2.5}$$

with $C_0, C_1 > 0$, uniformly for all $y \in \Gamma$. Here $A_0$ is an elliptic operator corresponding to the coefficient $a_0 = e^{a_0(x)}$, and $A$ is an elliptic operator corresponding to the coefficient $a = e^{a_M(y,x)}$. Hence, the weak formulation (2.4) again has a unique solution. Notice that in the log-additive case the solvability conditions 1) - 2) can be substantially relaxed, but this issue is beyond the scope of this paper.

### 2.2. Stochastic-Galerkin and stochastic-collocation discretizations

The *parametric weak equation* (2.4) can be reformulated as a variational equation in the tensor-product Hilbert space $V$. Introducing the corresponding 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

$$A_M(u_M, v) = \int_\Gamma \int_D f(x)v(y, x)dxdy =: b_M(v) \quad \forall\, v \in V. \tag{2.6}$$

**Lemma 2.1.** *([12]) Equation (2.6) is uniquely solvable in $V$.*

The variational formulation (2.6) gives rise to the stochastic-Galerkin approximation of sPDEs.

The method proposed in this paper also applies to the stochastic-collocation approximation method. We refer to [1] for detailed description of the stochastic-collocation method for elliptic sPDEs. We discretize the parametric equation (2.4) by the Galerkin FEM or Finite Differences (FD) methods in the physical domain $D$, and by the collocation method in the parameter domain $\Gamma$ (see §3.3 for more detail).

## 3. Collocation discretization in the parameter space

### 3.1. Formatted Tensor Representation of vectors and matrices

For the numerical solution of multiparameter problems, low-parametric representations of high-dimensional arrays (tensors) that arise from numerical discretizations of such equations will be used. It will be shown, that all computations required to solve a multiparametric problem will be reduced to fast operations with high-dimensional structured matrices and vectors. These representations (called tensor formats) are crucial to avoid curse of dimensionality.

In this paper, Tensor Train (TT) and (Quantics Tensor Train) (QTT) representations will be utilized heavily both for matrices and vectors (for detailed description see [22, 24, 23, 15, 12]), and for fast linear algebra operations in these formats TT-Toolbox[3] will be used.

The complexity of basic operations is greatly reduced. For example, to multiply an $n^d \times n^d$ matrix with TT-ranks $r_k \leqslant r$, by a vector of length $n^d$ with ranks $r'_k \leqslant r'$, the result is also a vector in TT-format with ranks bounded by $rr'$, and the complexity is linear in the dimension $d$ and polynomial in $n$ and ranks $r, r'$. The basic facts, notations, and algorithms for these formats are summarized in the next section.

[3]TT-Toolbox is publicly available from http://spring.inm.ras.ru/osel

### 3.2. Notations and basic facts about the TT and QTT formats

The basic objects used in this paper are multidimensional arrays, called tensors. They will be denoted by boldface letters, i.e., $\mathbf{A}$. Elements of a $n_1 \times n_2 \ldots \times n_d$ tensor $\mathbf{A}$ are denoted as $A(i_1, \ldots, i_d)$, and $n_k$ are referred to as *mode sizes*. Since tensors belong to a linear space, standard linear operations (addition, multiplication by a number) are naturally defined. The Frobenius norm of a tensor, $||\mathbf{A}||_F$ is defined as

$$||\mathbf{A}||_F = \sqrt{\sum_{i_1,\ldots,i_d} A(i_1, \ldots, i_d)^2}.$$

An important operation is *tensor-by-matrix multiplication* over the mode-$k$ (also called mode-product or contracted product). It is defined as

$$\mathbf{B} = \mathbf{A} \times_k U \quad \rightarrow \quad B(i_1, \ldots, i'_k, \ldots, i_d) = \sum_{i_k=1}^{n_k} A(i_1, \ldots, i_d) U(i_k, i'_k).$$

Tensors can be transformed into matrices in various ways. We adopt the following notation. Given a tensor $\mathbf{A} = A(i_1, i_2, \ldots, i_d)$ by

$$A(i_1 i_2 \ldots i_k; i_{k+1} \ldots i_d)$$

*k-th unfolding matrix* is denoted, i.e. first $k$ indices enumerate its rows, and last $d-k$ — its columns.

A detailed review of tensors and their application can be found in [17, 13].

A multidimensional array (tensor) $\mathbf{A} = [A(i_1, \ldots, i_d)]$, $(1 \leqslant i_k \leqslant n_k)$ is said to be in the TT (tensor train) format if it is represented as

$$A(i_1, i_2, \ldots, i_d) = \sum_{\alpha_1,\ldots,\alpha_{d-1}} G_1(i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \ldots G_d(\alpha_{d-1}, i_d), \tag{3.1}$$

where $\alpha_k$ varies from 1 to $r_k$, and $G_k$ are called *cores* of the TT-decompositions, and $r_k$ are called compression ranks, or simply TT-ranks of the decomposition. Two border cores of the TT-format are matrices. To make the decomposition more symmetric, it is natural to consider the *extended form*

$$A(i_1, i_2, \ldots, i_d) = \sum_{\alpha_0,\alpha_1,\ldots,\alpha_{d-1},\alpha_d} G_1(\alpha_0, i_1, \alpha_1) G_2(\alpha_1, i_2, \alpha_2) \ldots G_d(\alpha_{d-1}, i_d, \alpha_d), \tag{3.2}$$

where two dummy indices $\alpha_0$ and $\alpha_d$ are equal to one. This form simplifies the description of algorithms and will be used later on (corresponding ranks $r_0 = r_d = 1$).

Also, the $k$-th rank of the TT-decomposition of $\mathbf{A}$ will be denoted by $r_k(\mathbf{A})$. The TT-ranks are bounded from below by the ranks of unfolding matrices $A_k$,

$$rank(\mathbf{A}) \geqslant r_k \geqslant \operatorname{rank} A_k, \quad k = 1, ..., d.$$

The unfolding procedure is also called matrization of a tensor [3]. The inverse statement is also true: if $r_k = \operatorname{rank} A_k$, then there exists a TT-decomposition with these ranks [22], and, moreover, it can be computed by $d$ singular value decompositions (SVD) of auxiliary matrices

[23]. Moreover, such a procedure is stable: if the unfolding matrices are of approximate low-rank $r_k$:

$$A_k = R_k + E_k,$$

where $\operatorname{rank} R_k = r_k$ and $||E_k||_F = \varepsilon_k$, then TT-approximate $\mathbf{B}$, computed by a sequence of SVD decompositions, satisfies

$$\|\mathbf{A} - \mathbf{B}\|_F \leqslant \sqrt{\sum_{k=1}^{d-1} \varepsilon_k^2},$$

which confirms the stability of the approximation procedure (hereinafter called TT-SVD, since it can be considered as a generalization of SVD algorithm for matrices).

If all ranks are equal to $r$ and all mode dimensions are equal to $n$, then the TT-format requires $\mathcal{O}(dnr^2)$ memory cells. Hence, the storage is linear in $d$ and quadratic in $r$. The standard format to represent a $d$-dimensional array is the *canonical format*:

$$A(i_1, \ldots, i_d) \approx \sum_{\alpha=1}^{r} U_1(i_1, \alpha) \ldots U_d(i_d, \alpha). \tag{3.3}$$

It requires $\mathcal{O}(dnr)$ memory cells, however it suffers from certain drawbacks. Despite of the recent progress, there are no robust algorithms to compute a canonical decomposition numerically, and the approximation by a canonical tensor with a fixed rank can be ill-posed [6]. In contrast, computation of the best TT-approximation is a well-posed problem, and quasi-optimal approximation can be computed by means of the TT-SVD algorithm that uses standard LAPACK procedures, which is why it is preferable in numerical computations.

One of the most important procedures in the structured tensor computation is the *re-compression procedure*. Given a tensor $\mathbf{A}$ in the TT-format with non-optimal ranks $r_k$, we want to approximate it with another TT-tensor $\mathbf{B}$ with the smallest possible ranks $\widehat{r}_k \leqslant r_k$ while maintaining the desired relative accuracy $\varepsilon$:

$$||\mathbf{A} - \mathbf{B}||_F \leqslant \varepsilon ||\mathbf{B}||_F.$$

Such a projection will be denoted as

$$\mathbf{B} = T_\varepsilon(A).$$

The construction of such an operator in the canonical form is a notoriously difficult task, with no best solution known.

For the TT-format, it can be implemented by using a standard algorithm from linear algebra (SVD and QR decompositions). Such an algorithm is presented in [22]. For completeness of the presentation, we give it here (in a notation slightly different from [22]).

The MATLAB code for this algorithm is a part of TT-Toolbox. By $\mathrm{SVD}_\delta$ in Algorithm 1 we denote SVD with singular values that are set to zero if smaller than $\delta$, and by $\mathrm{QR}_{\mathrm{rows}}$ we denote the QR-decomposition of a matrix, where the $Q$ factor has orthonormal rows. The $\mathrm{SVD}_\delta(A)$ returns three matrices $U$, $\Lambda$, $V$ of the decomposition $A \approx U\Lambda V^\top$ (as a MATLAB **svd** function), and $\mathrm{QR}_{\mathrm{rows}}$ returns two: the $Q$-factor and the $R$-factor.

The complexity of the algorithm is $\mathcal{O}(dnr^3)$. All the basic operations of multilinear algebra (MLA): addition, multiplication by a number, scalar product, norm, matrix-by-vector

product can be implemented in TT-format. Together with the recompression procedure, this gives a nice tool for solving high-dimensional problems.

The QTT is a TT-decomposition applied to a special kind of tensors arising from the discretization of a certain function. It was considered for the tensorization of matrices ([23]) and vectors [12]. The simplest case is one-dimensional. Consider the function $f(x)$ of one variable, $x \in [a, b]$, and discretize it on a uniform grid with $2^d$ points:

$$v_k = f(x_k), \quad k = 1, \ldots, 2^d.$$

The corresponding vector can be reshaped into a $2 \times 2 \times \ldots \times 2$, $d$-dimensional tensor, to which TT-decomposition can be applied. It appears that for many functions the ranks $r_k$ are very small [12], which leads to a $\mathcal{O}(\log n)$ storage complexity for a vector of length $n$. Such an idea of introducing virtual dimensions can be generalized to higher dimensions. For example, for bivariate functions and their discretizations on a tensor grid, the corresponding tensor elements have the form

$$A(i_1, i_2, \ldots, i_d, j_1, \ldots, j_d), \quad 0 \leqslant i_k, j_k \leqslant 1.$$

**Algorithm 1** TT-recompression

**Require:** $d$-dimensional tensor $\mathbf{A}$ in the TT-format, required accuracy $\varepsilon$
**Ensure:** $\mathbf{B}$ in the TT-format with smallest possibles compression ranks $\widehat{r}_k$ such that

$$||\mathbf{A} - \mathbf{B}||_F \leqslant \varepsilon ||\mathbf{A}||_F, \quad i.e. \quad \mathbf{B} = T_\varepsilon(\mathbf{A}).$$

1: Let $G_k$, $k = 1, \ldots, d-1$ be cores of $\mathbf{A}$.
2: {Initialization}
Compute truncation parameter $\delta = \frac{\varepsilon}{\sqrt{d-1}} ||\mathbf{A}||_F$.
3: {Right-to-left orthogonalization}
4: **for** $k = d$ to 2 step $-1$ **do**
5: $[G_k(\beta_{k-1}; i_k \beta_k), R(\alpha_{k-1}, \beta_{k-1})] := \mathrm{QR}_{\mathrm{rows}}(G_k(\alpha_{k-1}; i_k \beta_k))$.
6: $G_{k-1} := G_k \times_3 R$.
7: **end for**
8: {Compression of the orthogonalized representation}
9: **for** $k = 1$ to $d - 1$ **do**
10: {Compute $\delta$-truncated SVD}
$[G_k(\beta_{k-1} i_k; \gamma_k), \Lambda, V(\beta_k, \gamma_k)] := \mathrm{SVD}_\delta[G_k(\beta_{k-1} i_k; \beta_k)]$.
11: $G_{k+1} := G_{k+1} \times_1 (V\Lambda)^\top$.
12: **end for**
13: Return $G_k$, $k = 1, \ldots, d$ as cores of $\mathbf{B}$.

TT-ranks crucially depend on the permutation of indices. For the two-dimensional case, it was found experimentally [12] (using the TT-SVD algorithm) that permutation of indices in the fashion

$$B(i_1 j_1, i_2 j_2, \ldots, i_d j_d),$$

i.e., with indices $i_k, j_k$ interleaved, is preferable. Some theoretical results on the approximation in the QTT-format were obtained in [12, 9].

To summarize, the QTT format for a $2^d \times 2^d \times \ldots \times 2^d$, $f$-dimensional arrays leads to a $\mathcal{O}(dfr^2)$ storage, and if $r$ is small, it is of logarithmic complexity in the total number of elements, $O(\log 2^{df})$, of the array (log-volume complexity).

Both the TT and the QTT formats can be also used for matrices with cores $G_k$ indexed by four indices $G_k(\alpha_{k-1}, i_k, j_k, \alpha_k)$ instead of three. For such a representation it is easy to implement a matrix-by-vector product, where both the matrix and the vector are in the TT (QTT) format.

Now, we will discuss how the QTT representation will be used for the discretization of parameter-dependent elliptic problems. A special structure of matrices can also be incorporated into cores $G_k$. For example, for sparse matrices in some modes the corresponding tensors $G_k$ will be sparse, and for diagonal dependence the corresponding cores will also be diagonal.

### 3.3. QTT representation of matrices and solution vectors

For each point $y \in \Gamma$ in the parameter space, we have an elliptic boundary value problem

$$\mathcal{A}(y, x)u(y, x) = f(x), \quad x \in D \in \mathbb{R}^{d_0},$$

which is discretized by a suitable approximation with $N$ degrees of freedom in the physical variable $x$. This yields a parametric linear system

$$A(y)v(y) = f, \quad f \in \mathbb{R}^N,\ v(y) \in \mathbb{R}^N, \quad y \in \Gamma. \tag{3.4}$$

The discretization can be performed by any suitable linear scheme (Galerkin, finite differences, projected collocation, etc.).

In the following, we apply the Galerkin collocation method. For each fixed $y \in \Gamma$, we discretize the parametric equation (2.4) by the Galerkin FEM via a set of piecewise linear hat functions $\{\phi_i\}$, $i = 1, ..., N$. The main problem is the dependence on the parameters $y = (y_1, \ldots, y_M)$. For each $m, 1 \leqslant m \leqslant M$, a one-dimensional grid of collocation points $\Gamma_m = \{y_m^{(k)}\} \in [-1, 1]$, $k = 1, \ldots, n$ is introduced. This is equivalent to the collocation method applied to (3.4), and the problem is reduced to $n^M$ linear systems

$$A(j_1, \ldots, j_M)u(j_1, \ldots, j_M) = f, \quad 1 \leqslant j_k \leqslant n,$$

which can be written as one large linear system

$$\mathbb{A}\mathbf{u} = \mathbf{f}, \tag{3.5}$$

where $\mathbb{A}$ is an $Nn^M \times Nn^M$ matrix, $\mathbf{u}$ and $\mathbf{f}$ are vectors of length $Nn^M$.

In the *additive case* the parameter-dependent matrix takes the form

$$A(y) = A_0 + \sum_{m=1}^{M} A_m y_m, \quad y \in \Gamma_M := \Gamma_m^M,$$

where $A_m$ are $N \times N$ matrices and $N$ is the number of degrees of freedom of discretization in $x$. In this case, $\mathbb{A}$ can be represented in the tensor form

$$\mathbb{A} = A_0 \times I \times \ldots \times I + A_1 \times D_1 \times I \times \ldots \times I + \ldots + A_M \times I \times \ldots \times D_M, \tag{3.6}$$

where $D_m$, $m = 1, \ldots, M$, is an $n \times n$ diagonal matrix with positions of collocation points $\{y_m^{(k)}\}$, $k = 1, \ldots, n$ on the diagonal, and the right-hand side has a tensor rank 1

$$\mathbf{f} = f \times e \times \ldots \times e,$$

where $e$ is a vector of all ones of length $n$.

The same approach can also be used for the *log-additive case*. The resulting linear system also has the form (3.4) - (3.5), but the dependence on $y$ is no longer affine and special techniques should be used for the matrix approximation in the $M$-dimensional parameter space.

In the log-additive case, system (3.5) has a similar form, but there will be no straightforward low tensor rank representation to the matrix $\mathbb{A}$ like (3.6). However, a still good low-rank approximations of the form

$$\mathbb{A} \approx \sum_{k=1}^{R} \bigotimes_{m=0}^{M} A_{mk},$$

where matrices $A_{mk} \in \mathbb{R}^{(M+1)\times n}$, will be precomputed and utilized for fast calculations.

It is natural to consider low-parametric tensor formats for the solution $\mathbf{u}$, which can be regarded as an $(M+1)$-dimensional tensor. Several options are available. A numerical solution of high-dimensional sPDEs in canonical format was considered [16]. Preliminary application of the hierarchical Tucker format was addressed in [18].

In this paper, we apply the QTT format to represent high-dimensional tensors in parametric variables. This representation gives a log-volume complexity in the number of elements of a tensor for several important problems. It has all basic linear algebra operations implemented in MATLAB, and it can be used effectively for solving equations of the form (3.5) by structured iterations with QTT-truncations as described in Section 4.

For the additive case, the rank-$(M+1)$ representation of the matrix $\mathbb{A}$ is available at no cost. For the log-additive case, it is very difficult to obtain canonical approximation to $\mathbb{A}$. However, QTT approximation to $\mathbb{A}$ can be computed by a certain fast procedure with recompression at each step. This procedure will be described in the next section.

We show that in some cases enhanced numerical algorithms can be designed using the localized version of the QTT and canonical formats.

### 3.4. Matrix approximation in the log-additive case

Let us describe how to compute a low-parametric representation for a matrix in the log-additive case for a model one-dimensional example. Suppose $D$ is $[0, 1]$ and the Galerkin discretization in $x$ gives

$$A(i, j, y) = \int_D b(y, x) \frac{\partial \phi_i}{\partial x} \frac{\partial \phi_j}{\partial x} dx, \quad y \in \Gamma, \quad D = [0, 1]. \tag{3.7}$$

As basis functions, take the standard piecewise-linear hat functions $\{\phi_i\}$, $i = 1, ..., N$, and also apply simple quadratures to integrals (3.7). This gives (up to a factor $h^2$) a three-diagonal matrix $A(y)$ with elements

$$\begin{aligned} A(i, i, y) &= \frac{1}{4}(b(y, x_{i-1}) + 2b(y, x_i) + b(y, x_{i+1})), \\ A(i, i-1, y) &= \frac{1}{2}(b(y, x_{i-1}) + b(y, x_i)), \\ A(i-1, i, y) &= A(i, i-1, y), \end{aligned}$$

for $i = 1, ..., N$, and $y \in \Gamma$. Recall that

$$b(y, x) = e^{a_M(y,x)} = e^{a_0(x)} \prod_{m=1}^{M} e^{a_m(x) y_m}.$$

Hence, it is easy to represent the matrix $A(y)$, $y \in \Gamma$ in the low tensor rank format,

$$A(y) = D(y) + Z(y) + Z^\top(y),$$

where $D(y)$ is a diagonal of $A$, $Z$ is the first subdiagonal. First, consider $D(y)$. It can be represented as

$$D(y) = \sum_{i=1}^{N} A(i, i, y) e_i e_i^\top = \frac{1}{4}(C_1(y) + 2C_2(y) + C_3(y)),$$

where $C_2(y)$ can be written in the form

$$C_2(y) = \sum_{i=1}^{N} e_i e_i^\top e^{a_0(x_i)} \prod_{m=1}^{M} e^{a_m(x_i) y_m}. \tag{3.8}$$

After taking $C_2(y)$ at collocation points $y \in \Gamma_M$ a diagonal matrix of size $Nn^m \times Nn^m$ appears, and it is easy to see that each summand in (3.8) has a tensor rank-1. Moreover, if the QTT format is considered in variable $y_m$, then the TT-ranks will be equal to 1, since it is an exponential function [12]. This proves the following result.

**Lemma 3.1.** *For quadrature discretization of a 1d PDE in the log-additive case each element* $\mathbf{A}(i, j, y)$ *has a canonical decomposition of a rank not larger than* 3*. The same QTT-rank bound holds true.*

This gives rise to a new format (local low-rank approximation [13]) for representing a tensor. This format can be used directly to represent the matrix $\mathbb{A}$: each non-zero entry of the matrix is represented as a low-rank $M$-dimensional tensor. The full QTT-rank can also be estimated as in the following Lemma 3.2.

As a consequence of Lemma 3.1, we conclude that $C_2(y)$ has rank $N$ at most. The ranks of matrices $C_1, C_3$ are also bounded by $N$. For $Z(y) = \frac{1}{2}(C_1(y) + C_2(y))$, we have two quadrature points, so the rank bound is $2N$, the same holds for $Z^\top(y)$, and the total rank estimate is $(1 + 1 + 1 + 2 + 2)N = 7N$. This estimate uses the fact that any fixed matrix element $f(y) = A(i, j, y)$ considered as an $M$-dimensional tensor has a canonical rank bounded by a small constant, and there are only $\mathcal{O}(N)$ nonzero elements. This leads to the following result.

**Lemma 3.2.** *For quadrature discretization of a 1d PDE in the log-additive case their exists a rank-R canonical approximation to the assembled matrix* $\mathbb{A}$ *with the rank estimate*

$$R \leqslant 7N, \tag{3.9}$$

*uniformly in* $n$ *and* $M$*.*

The arguments of Lemmas 3.1 and 3.2 also apply to an arbitrary space dimension in the physical variable $x \in \mathbb{R}^{d_0}$.

**Remark 3.1.** Similar arguments prove that

$$rank(A(i,j,y)) \leqslant C3^{d_0} \quad \text{and} \quad rank(\mathbb{A}) \leqslant C3^{d_0}N,$$

with constant $C$ independent of $N$, $n$ and $M$. Consequently, the QTT ranks of the corresponding local matrices scale as $O(3^{d_0})$.

For a one-dimensional problem with small grids (of the order of hundreds) it already gives a nice representation. However, for a two-dimensional physical problem, $N$ grows quadratically in the one-dimensional grid size and estimate (3.9) gives very large values of ranks.

In practice the ranks are usually much smaller, normally in the range $O(M)$, and the canonical representation with an overestimated rank $R$ can be compressed by the canonical-to-QTT compression algorithm [23] to the QTT-format. The algorithm is just the addition of rank-one terms comprising the decomposition one-by-one and compressing the result afterwards to avoid an excessive rank increase. This simple scheme allows fast computation of the low-rank optimized TT-approximation to the matrix $\mathbb{A}$. It is summarized in Algorithm 2.

Recently in [5] it was shown that under some mild assumptions in the additive case the mapping $u(y,x)$ for each fixed $x$ is an analytic function of $y$ and there exists a small-degree polynomial approximation to it. As a consequence, here comes a canonical rank estimate $C|\log\varepsilon|^{M-1}$, which is nice for small $M$, but still grows exponentially in $M$. However, as our numerical experiments demonstrate, this estimate is too pessimistic. Actually, the rank bound for the solution appeares to be almost uniform in $M$.

## 4. Preconditioned QTT-truncated iteration

The QTT format can be used effectively for solving equations of form (3.5) by structured iterations with QTT-truncations of the form

$$\widetilde{\mathbf{u}}^{(m+1)} := \mathbf{u}^{(m)} - \omega\mathbb{B}_m\left(\mathbb{A}\mathbf{u}^{(m)} - \mathbf{f}\right), \quad \mathbf{u}^{(m+1)} = T_\varepsilon(\widetilde{\mathbf{u}}^{(m+1)}) \to \mathbf{u}, \tag{4.1}$$

where $T_\varepsilon$ is the rank truncation operator preserving accuracy $\varepsilon$.

At each step, the TT-ranks increase and have to be reduced by the recompression procedure from [22]. The procedure will work if the solution can indeed be approximated in the TT format, and we will verify this numerically for several examples later on.

In the additive case of stochastic PDEs, a good choice of a preconditioner is the rank-1 tensor

$$\mathbb{B}_0 = A_0^{-1} \times I \times \ldots \times I,$$

(see [16]), which is easy to incorporate into the TT-framework. The spectral equivalence for this preconditioner is proved in [16].

However, in a more general setting, the efficient preconditioner has to be chosen adaptively to the current iterand living in the parametric space without any prior knowledge. At each iteration the correction equation has to be solved approximately

$$\mathbb{A}\mathbf{c} \approx \mathbf{f} - \mathbb{A}\mathbf{u},$$

or in terms of the (nonlinear) preconditioner $\mathbb{B}$,

$$\mathbf{c} = \mathbb{B}(\mathbf{f} - \mathbb{A}\mathbf{u}).$$

**Algorithm 2** Matrix approximation in the log-additive case

**Require:** Subroutine that computes any element of the matrix $A(i,j,y)$, $1 \leqslant i,j \leqslant N$ in the QTT-format in the stochastic variable $y = (y_1, \ldots, y_M)$, with $2^p$ points in each stochastic mode, truncation parameter $\varepsilon$.

**Ensure:** QTT-approximation to the matrix $\mathbb{A}$

1: Let $\mathcal{S}$ be a sparsity pattern of $A$.
2: $\mathbf{A} := 0, M := 0$
3: **for** $(i,j) \in \mathcal{S}$ **do**
4: $\mathbf{B} := A(i,j,y)$ in the QTT-format with cores $B_2, \ldots, B_{Mp+1}$
5: {Concatenate tensors $\mathbf{A}$ and $\mathbf{B}$ }
6: $r_k = r_k(\mathbf{A}), \widehat{r}_k = r_k(\mathbf{B})$, $A(1:M,:) = \mathbf{A}, A(M+1,:) = \mathbf{B}$ by concatenating cores:
7: $A_1 := \begin{pmatrix} A_1 & 0_{M \times \widehat{r}_1} \\ 0_{1 \times r_1} & 1_{1 \times \widehat{r}_1} \end{pmatrix}$.
8: **for** $k = 2$ to $Mp+1$ **do**
9: $C_k := 0_{(r_{k-1}+\widehat{r}_{k-1}) \times m_k \times (r_k + \widehat{r}_k)}$.
10: $C_k(1 : r_{k-1}, :, 1 : r_k) := A_k$
11: $C_k(r_{k-1}+1 : \widehat{r}_{k-1}, :, r_k + 1 : \widehat{r}_k) := B_k$.
12: $A_k := C_k$.
13: **end for**
14: $\mathbf{A} := T_\varepsilon(\mathbf{A})$.
15: **end for**
16: {How to treat the result}
$\mathbf{A}$ is an $\mathrm{nnz} \times 2 \times \ldots \times 2$ dimensional tensor with $(Mp+1)$ dimensions
— "sparse" representation of $\mathbb{A}$
The first core of $\mathbf{A}$, $A_1$ is now an $\mathrm{nnz} \times r_1$ matrix, where nnz is the number of nonzeros in the sparsity pattern of $\mathbb{A}$. Each column of $A_1$ corresponds to the $N \times N$ sparse matrix, and this is the sparse representation of the first core of $\mathbb{A}$. The other cores of $\mathbb{A}$ are diagonal matrices formed from the cores of $\mathbf{A}$ (for each core of size $r_{k-1} \times 2 \times r_k$, a tensor of size $r_{k-1} \times 2 \times 2 \times r_k$ is formed).
17: {Complexity}
The complexity of the algorithm is $\mathcal{O}(NMpr^3)$.

To implement $\mathbb{B}$, we propose to use a *one-point preconditioner scheme*, i.e., precondition by the parameter-independent $N \times N$ matrix $A(y^*)$ for some special choice of the multiparameter $y^*$:

$$\mathbf{c} = A(y^*)^{-1}(\mathbf{f} - \mathbb{A}\mathbf{u}).$$

This solves exactly only one of our systems, and $y^*$ should be selected adaptively. As a simple heuristics, the following scheme is proposed. For the residue tensor, $v(x,y) = \mathbf{f} - \mathbb{A}\mathbf{u}$, $x \in \mathbb{R}^N$, $y \in \Gamma_M$, we can find an approximate maximal element, where the residual is small, using multidimensional generalization of the maxvol algorithm [8]. This procedure is fast and inexpensive for a low-rank TT-tensor (it has complexity $\mathcal{O}(Nr^2 + pMr^3)$, as a result, we have the position of the maximum, $(x^*, y^*)$ and use $A(y^*)$. We notice that a more natural approach is to compute the norms of all residuals in $x$ for each $y$, and then compute the maximum. This procedure is more robust but more expensive computationally, and, surprisingly, in our experiments it usually gave a worse convergence. Notice that the preconditioner $\mathbb{B}_0$ corresponds to the choice $y^* = 0$ in terms of the continuous variable $y$.

Once $y^*$ has been found the preconditioner is defined by

$$\mathbb{B} = A(y^*)^{-1} \times I \times \ldots \times I.$$

This is a nonlinear preconditioner, since $y^*$ is determined adaptively at each step, so not every linear solver can be used: the only option beyond the Richardson iteration is the geometric version of GMRES. To apply $\mathbb{B}$ to the TT-vector, one has to solve $r$ independent $N \times N$ linear systems, where $r$ is the first TT-rank of the vector. For elliptic problems any suitable fast solver can be used. Our examples are two-dimensional, so a fast direct solver for sparse matrices can be applied. By $\mathbf{Solve}(N, r)$ we denote the complexity to solve a linear system of the form

$$A(y^*)V = F_j, \quad j = 1, ..., r.$$

Finally, the solution algorithm looks as follows (the numerical complexity of respective steps in Algorithm 3 is specified in the right column).

## 5. Numerical experiments

### 5.1. Matrix approximation

We present numerical results for the approximation of the full system matrix in the QTT format. For the additive case, the ranks grow linearly in $M$. For the log-additive case, no results are known, and we present the first numerics for the approximation of the full matrix corresponding to certain log-additive model examples.

Consider a 2D-dimensional SPDE in stratified media (i.e., with the coefficient depending on the 1D variable) in the two cases:

1. Polynomial decay: $a_m(x) = \dfrac{0.5}{(m+1)^2} \sin mx$, $x \in [-\pi, \pi]$, $m = 1, \ldots, M$.

2. Exponential decay: $a_m(x) = e^{-0.7m} \sin mx$, $x \in [-\pi, \pi]$, $m = 1, \ldots, M$.

The parametric space is discretized on a uniform mesh in $[-1, 1]$ with $2^p$ points in each spatial direction. For the experiments, $p = 8$ is taken.

The ranks are presented with different truncation parameters. Table 5.1 presents the results for the log-additive case and polynomial decay of coefficients, and Table 5.2 — for exponential decay. The dependence on $M$ is linear for polynomial decay, and seems to be much milder in the case of exponential decay, which is rather natural.

Table 5.3 describes the dependence on the accuracy for a fixed $M$. This confirms that the ranks are logarithmic in accuracy $\varepsilon$.

Table 5.1. **Rank-dependence of the matrix in the QTT format, 2D SPDE, log-additive case, polynomial decay** $N = 128$, $p = 8$

| M | QTT-rank($10^{-7}$) | QTT-rank($10^{-3}$) |
|---|---|---|
| 5 | 27 | 10 |
| 10 | 44 | 17 |
| 20 | 78 | 27 |
| 40 | 117 | 49 |

Table 5.2. **Dependence of the matrix QTT rank on** $M$**. 2D SPDE, log-additive case, exponential decay,** $N = 128$, $p = 8$

| M | QTT-rank($10^{-7}$) | QTT-rank($10^{-3}$) |
|---|---|---|
| 5 | 33 | 11 |
| 10 | 43 | 21 |
| 20 | 51 | 23 |
| 40 | 50 | 25 |

**Algorithm 3** Richardson iteration with a 1-point preconditioner

**Require:** The right-hand side $f$ in the QTT-format ($f$ can be considered as a $N \times 2 \times 2 \times \ldots \times 2$ $(1 + Mp)$-dimensional tensor), the block-diagonal matrix $\mathbb{A} = \mathbb{A}(i, i', j_1, j_2, \ldots, j_{Mp})$, $i, i' = 1, \ldots, N$, $j_k = 1, 2$, $k = 1, \ldots, Mp$ in the QTT-format, the truncation parameter $\varepsilon$, the number of iterations $n_{\text{it}}$.

**Ensure:** Approximate solution $x$ in the QTT-format of the equation $\mathbb{A}x = f$.

1: {Initialization} $x = 0$

2: **for** $k = 1$ to $n_{\text{it}}$ **do**

3: {Compute residual}
$\mathbf{res} = T_\varepsilon(\mathbb{A}x - f)$ $\quad \mathcal{O}(N(r_1(x)r_1(\mathbb{A}))^2 + \sum_{m=2}^{Mp} r_m^2(x) r_m^2(\mathbb{A}))$
**res** is represented in the QTT format:
$\mathbf{res}(i, j_1, \ldots, j_{Mp}) = \sum_{\alpha_1, \ldots, \alpha_{Mp}} R_1(i, \alpha_1) R_2(\alpha_1, j_1, \alpha_2) \ldots R_{Mp+1}(\alpha_{Mp}, j_{Mp})$

4: {Maximal residue}
$[i^*, j_1^*, j_2^*, \ldots j_{Mp}^*] = \arg\max |\mathbf{res}(i, j_1, j_2, \ldots, j_{Mp})|$ $\quad \mathcal{O}(Nr_1^2(\mathbf{res}) + \sum_{m=2}^{Mp} r_m^3(\mathbf{res}))$

5: {1-point preconditioner}
Compute $N \times N$ sparse matrix $B$ as
$B = A(i, i', j_1^*, \ldots, j_{Mp}^*)$
by contracting $\mathbb{A}$ over stochastic modes $\quad \mathcal{O}(Nr_1(\mathbb{A}) + \sum_{m=2}^{Mp} r_m^2(\mathbb{A}))$

6: {Apply the precondioner}
Solve for $BR' = R_1$, where $R_1$ is the first core of **res** using any suitable solver in the physical space. $\quad \mathbf{Solve}(N, r_1(\mathbf{res}))$

7: Set the first core of **res** to $R'$

8: $x := x + \mathbf{res}$

9: $x := T_\varepsilon(x)$ $\quad \mathcal{O}(Nr_1^2(x) + \sum_{m=2}^{Mp} r_m^3(x))$

10: **end for**

Table 5.3. **Dependence of the matrix QTT-rank on the accuracy. 2D SPDE, log-additive case, exponential decay,** $N = 128$**,** $M = 40$**,** $p = 8$

| $\varepsilon$ | QTT-rank($\varepsilon$) |
|---|---|
| $10^{-3}$ | 25 |
| $10^{-4}$ | 31 |
| $10^{-5}$ | 38 |
| $10^{-6}$ | 44 |
| $10^{-7}$ | 50 |

Tables 5.1 – 5.3 confirm numerically that the matrices for the log-additive case have low maximal QTT-ranks, and this representation can be used for the solution. In what follows two-dimensional model examples will be considered (i.e., $d_0 = 2$), for both the additive and the log-additive cases, as well as two multi-parameter problems will be studied.

We use two different TT rank estimates for tensors: one characterising the overall storage needs and complexity, $\hat{r}_{TT}$, and the other one serving for the QTT-rank disctribution, $\overline{r}_{QTT}$:

$$\hat{r}_{TT}(\mathbf{u}) = \sqrt{\frac{\sum n_i r_i r_{i+1}}{\sum n_i}}, \quad \overline{r}_{QTT}(\mathbf{u}) = \sqrt{\frac{1}{M} \sum r_i r_{i+1}}.$$

### 5.2. Additive case

As the first example, consider the two-dimensional diffusion in stratified media with the diffusion coefficient

$$a(x_1, x_2, y_2, \ldots, y_M) = 1 + \frac{1}{2}\sum_{m=2}^{M} \lambda_m \sin(mx_1) y_m, \tag{5.1}$$

where $\lambda_m = e^{-0.7m}$. The results are presented in Fig. 5.1 - 5.3.

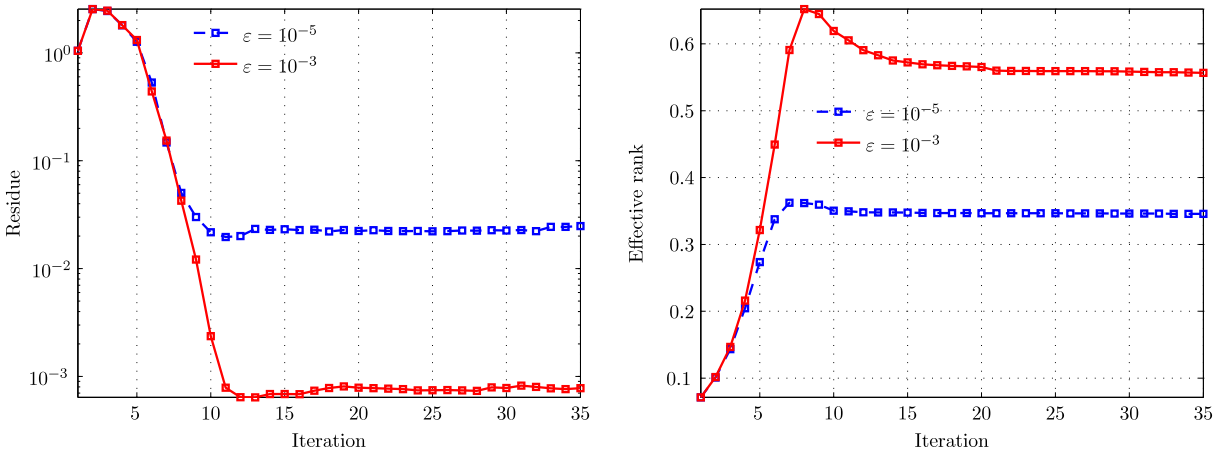



Fig. 5.1. Convergence in the stratified 2D additive example with two different truncation parameters, 1-point preconditioner. Left: Residue with iteration; Right: $\hat{r}_{QTT}$-ranks with iteration, $M = 40$

The time dependence on $M$ is presented in Fig. 5.2. The rank dependence on $M$ in the solution is presented in Fig. 5.3.

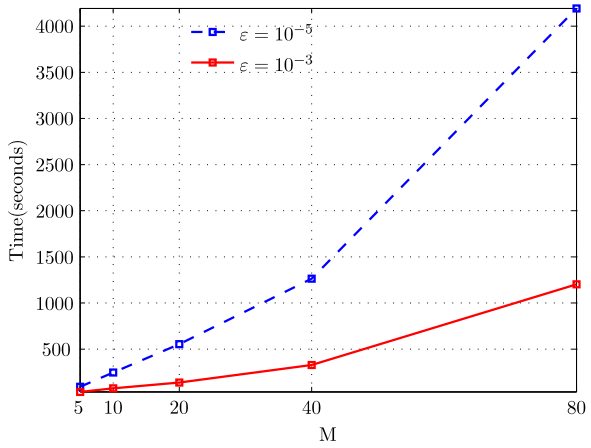



Fig. 5.2. Time for 35 iterations, additive case, example (5.1)

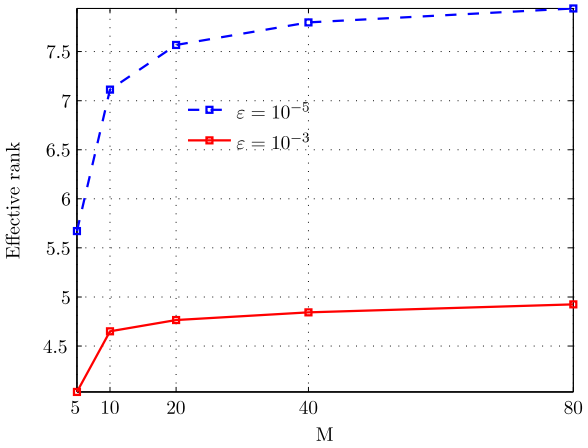


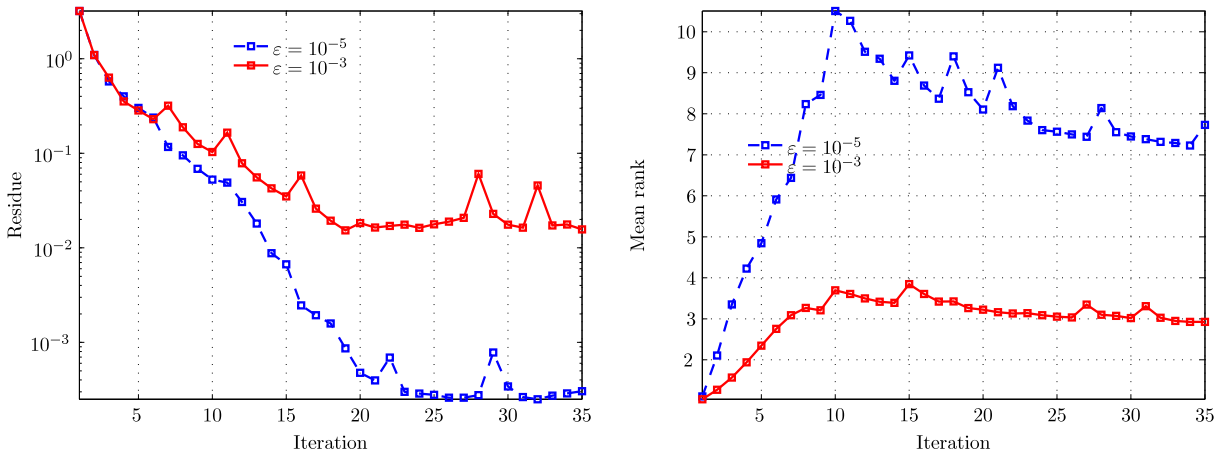

Fig. 5.3. $\overline{r}_{QTT}$-ranks of the solution vs. $M$, additive case, example (5.1)

### 5.3. Log-additive case

As the second example, we consider the two-dimensional diffusion in stratified media with the diffusion coefficient

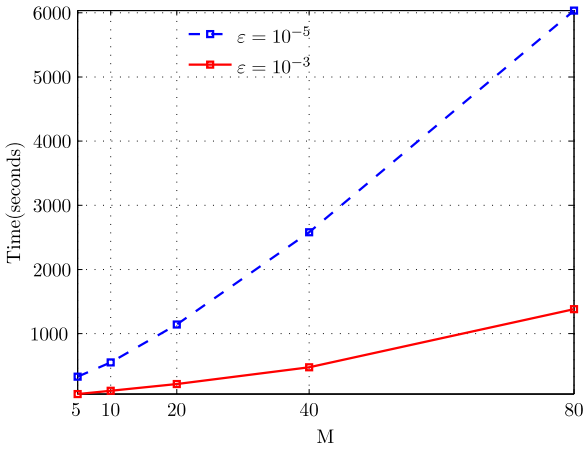
$$a(x_1, x_2, y_2, \ldots, y_M) = \exp(1 + \sum_{k=2}^{M} \lambda_k \sin(kx_1) y_k), \tag{5.2}$$

where $\lambda_k = e^{-0.7k}$. The results are presented in Fig. 5.4.




F i g. 5.4. Convergence in the stratified 2D log-additive example with two different truncation parameters, 1-point preconditioner. Left: Residue with iteration; Right: $\overline{r}_{QTT}$-Ranks with iteration, $M = 40$

The time dependence on $M$ is presented in Fig. 5.5




F i g. 5.5. Time for 35 iterations, log-additive case, example (5.2)

## 5.4. Multiparameter problems

In this subsection, two "deterministic" problems with several parameters will be considered. The first one, borrowed from [2], is as follows. Again, we consider the diffusion equation

$$\mathrm{div}_x\left(a(y,x)\mathrm{grad}_x u\right) = f \in L^2(D), \quad y \in \Gamma,$$

in a square $D = [0,1]^2$, where the diffusion coefficient is represented as

$$a(x,y) = 1 + \sum_{i=1}^{4} \gamma_i \xi_i(x) y_i,$$

with $\xi_i(x)$ being the indicator function of four disks (see Fig. 5.6), and $y_i \in [-0.99, 0]$, $i = 1, \ldots, 4$.

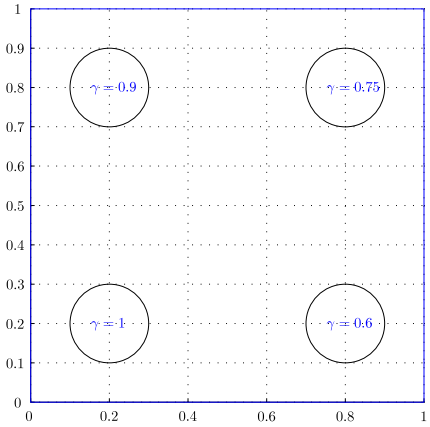



Fig. 5.6. 4-circles test problem

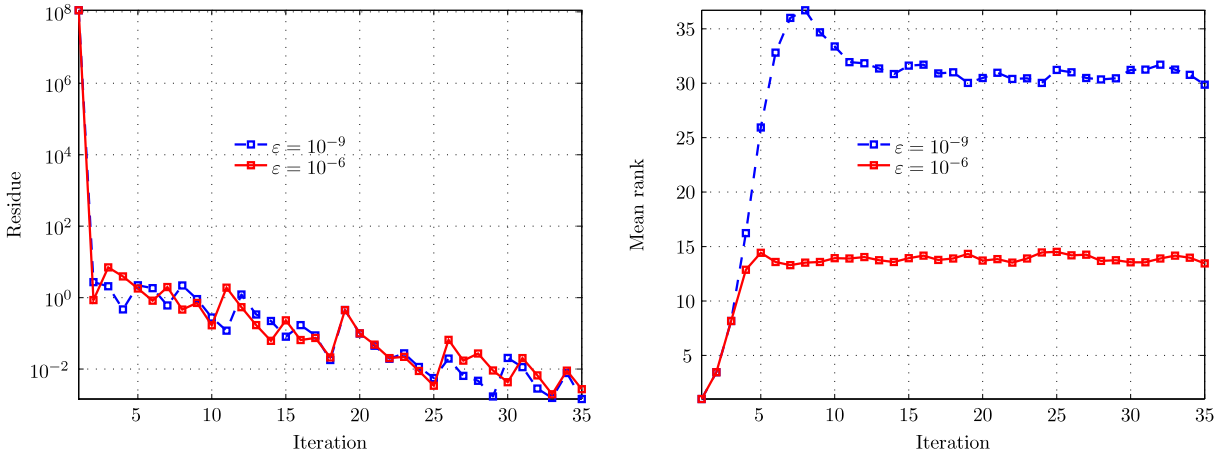



Fig. 5.7. Convergence in the 4-circles example with two different truncation parameters, 1-point preconditioner, Left: Residue with iteration, Right: Ranks with iteration

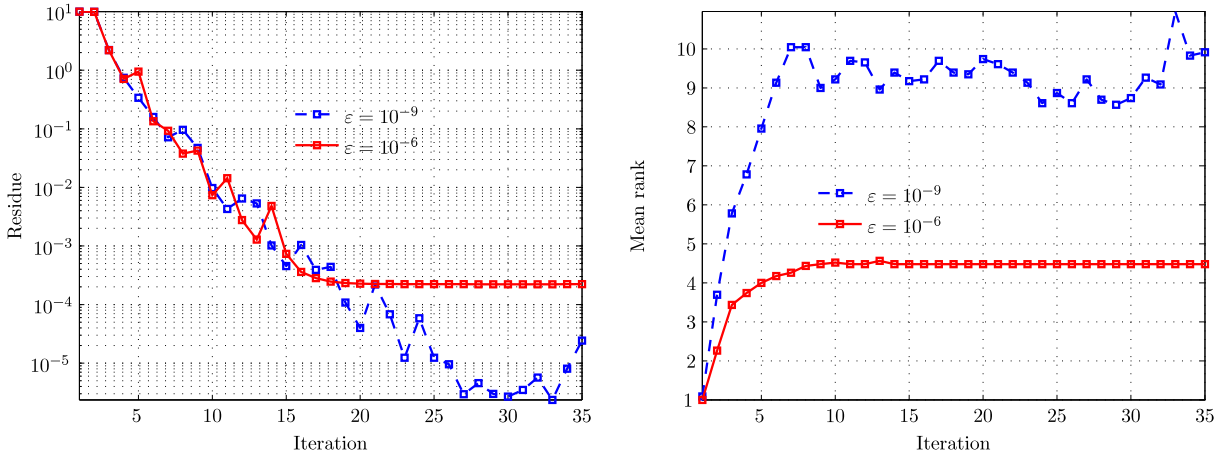
The average time for one iteration was 0.22 seconds for the truncation parameter $\varepsilon = 10^{-6}$ and 0.64 seconds for $\varepsilon = 10^{-9}$.

The second problem is the stationary heat equation from Oberwolfach benchmarks (see [25]), considered in [18], whose matrix form is as follows:

$$A_0 u + (A_1 y_1 + A_2 y_2 + A_3 y_3) u = -b,$$

with $A_i, i = 1, \ldots, 4$ are $4257 \times 4257$ matrices, $b$ is a vector of length 4257, and $A_1, A_2, A_3, A_4$ refer to different boundary conditions. This is related to the boundary condition independent modelling [25], and such problems appear in compact thermal modelling ([11]). The parameters $y_i$ vary from $10^8$ to $10^9$.

The average time for one iteration was 0.22 seconds for the truncation parameter $\varepsilon = 10^{-6}$ and 0.64 seconds for $\varepsilon = 10^{-9}$.




F i g. 5.8. Convergence in the Oberwolfach example with two different truncation parameters, 1-point preconditioner, Left: Residue with iteration, Right: Ranks with iteration

## 6. Conclusions

We have presented the first application of the QTT format to the solution of high-dimensional equations arising in stochastic PDEs and in parameter-dependent elliptic equations. We have proved that in both the additive and the log-additive cases the ranks in the QTT matrix format are bounded by a constant independent of $M$. However, it depends on $N$ – the physical problem size. The proof of the rank estimate is constructive and gives rise to an approximation algorithm that is free of the "curse of dimension". Using this algorithm, we have shown by numerical experiments that the estimate is rather pessimistic – actually the ranks scale linearly in $M$ in the worst case, and linearly in $|\log \varepsilon|$, where $\varepsilon$ is the accuracy of approximation. A similar rank behaviour is observed for the solution of the equation. To solve the equation, we use QTT-truncated iteration with the adaptive block-Jacobi-like preconditioner, which demonstrated the linear convergence rate in our numerical experiments. To summarize, the proposed method looks promising for the approximation and solution of parameter-dependent equations in the case of the additive and log-additive coefficient dependence on parameters.

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