

Efficient low-rank approximation of the stochastic Galerkin matrix in tensor formats

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In this article we describe an efficient approximation of the stochastic Galerkin matrix which stems from a stationary diffusion equation. The uncertain permeability coefficient is assumed to be a log-normal random field with given covariance and mean functions. The approximation is done in the canonical tensor format and then compared numerically with the tensor train and hierarchical tensor formats. It will be shown that under additional assumptions the approximation error depends only on smoothness of the covariance function and does not depend either on the number of random variables nor the degree of the multivariate Hermite polynomials.

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1 Introduction

The particular problem considered here is formally a stationary diffusion equation described by an uncertain conductivity parameter. Let $D \subset \mathbb{R}^d$ be a compact domain and $(\Omega, \mathcal{A}, \mathbb{P})$ a probability space. The diffusion problem is given by

$$\left. \begin{aligned} -\operatorname{div}(\kappa(\omega, x)\nabla u(\omega, x)) &= f(\omega, x) && \text{for all } x \in \dot{D} \\ u(\omega, x) &= 0 && \text{for all } x \in \partial D \end{aligned} \right\} \text{a.s. in } \omega \in \Omega, \quad (1)$$

where the conductivity κ and the source term f are random fields over $\Omega \times D$.

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The weak formulation of (1) reads as follows (see e.g. [8, 19, 18]): Find $u \in L^2(\Omega; H_0^1(D))$ such that for all $v \in V$

$$\mathbf{a}(u, v) := \int_{\Omega} \int_D \kappa(\omega, x) \nabla u(\omega, x) \cdot \nabla v(x) dx d\mathbb{P}(\omega) = \int_{\Omega} \int_D f(\omega, x) v(x) dx d\mathbb{P}(\omega), \quad (2)$$

where V denotes the space of test functions and must be chosen appropriately. A general issue with this formulation arises if κ is not essentially bounded nor away from zero over the entire $\Omega \times D$. Nevertheless, in [22] or [10] it is shown that under additional assumptions to the right-hand side f and special choices of V the weak formulation is well-posed.

In order to solve (1) numerically, one has to perform its full discretisation, in both the deterministic and stochastic spaces. The method of choice is the stochastic Galerkin discretisation, see e.g. [21, 16, 8, 20, 2, 15, 29].

Our considerations are based on the following assumption on the conductivity κ .

Assumption 1. *There exists a Gaussian random field γ over $\Omega \times D$ such that $\kappa = \exp \gamma$. $\kappa(\cdot, x) \in L^2(\Omega)$ holds for every $x \in D$. The mean function $m_{\kappa}(x) := \mathbb{E}(\kappa(\cdot, x))$ and the covariance function*

$$\Gamma_{\kappa}(x, y) := \text{cov}(\kappa(\cdot, x), \kappa(\cdot, y)) = \mathbb{E}[(\kappa(\cdot, x) - m_{\kappa}(x))(\kappa(\cdot, y) - m_{\kappa}(y))]$$

are given as continuous functions over D resp. $D \times D$.

The mean and covariance functions of κ determine the mean and covariance functions of γ entirely, since

$$\Gamma_{\gamma}(x, y) = \ln [\Gamma_{\kappa}(x, y) + m_{\kappa}(x)m_{\kappa}(y)] - \ln [m_{\kappa}(x)m_{\kappa}(y)], \quad (3)$$

$$m_{\gamma}(x) = 2 \ln m_{\kappa}(x) - \frac{1}{2} \ln [\Gamma_{\kappa}(x, x) + m_{\kappa}(x)^2]. \quad (4)$$

Both random fields are elements in $L^2(\Omega \times D)$.

Let \mathcal{C}_{κ} and \mathcal{C}_{γ} be the integral operators on $L^2(D)$ with kernels Γ_{κ} and Γ_{γ} respectively. Since the kernels are continuous and the domain D is compact, these operators are Hilbert-Schmidt operators. It exists an orthonormal basis $\kappa_1, \kappa_2, \dots \in L^2(D)$ of eigenfunctions and a sequence of associated eigenvalues $\lambda_1 \geq \lambda_2 \geq \dots \geq 0$ of \mathcal{C}_{κ} such that $\mathcal{C}_{\kappa}\kappa_l = \lambda_l\kappa_l$ for all $l \in \mathbb{N}$.

Accordingly, $\gamma_1, \gamma_2, \dots \in L^2(D)$ denote the orthonormal basis of eigenfunctions and $\lambda'_1 \geq \lambda'_2 \geq \dots \geq 0$ are the corresponding eigenvalues of \mathcal{C}_{γ} . The functions $\theta_k(\omega) = \frac{1}{\lambda'_k} \int_D (\gamma(\omega, x) - \bar{\gamma}(x)) \gamma_k(x) dx$ for those $k \in \mathbb{N}$, where $\lambda'_k > 0$ are jointly normal distributed and orthonormal random variables in $L^2(\Omega)$. Here $\bar{\gamma}(x)$ denotes the mean value of $\gamma(\omega, x)$. If $\gamma(\omega, x)$ is centred, then $\bar{\gamma}(x) = 0$. We shall write $\boldsymbol{\theta}$ as a short hand for the sequence consisting of these $\theta_1, \theta_2, \dots$.

Let $(\mathbb{N}_0)_{\mathcal{C}}^{\mathbb{N}} := \{(\alpha_1, \alpha_2, \dots) \in (\mathbb{N}_0)^{\mathbb{N}} \mid \exists K \in \mathbb{N} \forall k \geq K : \alpha_k = 0\}$ be the set of sequences in \mathbb{N}_0 with only finitely many nonzero elements. For $\boldsymbol{\iota} \in (\mathbb{N}_0)_{\mathcal{C}}^{\mathbb{N}}$ we set $H_{\boldsymbol{\iota}}(\mathbf{x}) = \prod_{k=1}^{\infty} h_{\iota_k}(x_k)$ for $\mathbf{x} \in \mathbb{R}^{\mathbb{N}}$, where h_{ι} denotes the ι -th Hermite polynomial. The $H_{\boldsymbol{\iota}}$ are called multivariate Hermite polynomials and $\{\frac{1}{\sqrt{\boldsymbol{\iota}!}} H_{\boldsymbol{\iota}}(\boldsymbol{\theta}) \mid \boldsymbol{\iota} \in (\mathbb{N}_0)_{\mathcal{C}}^{\mathbb{N}}\}$ is an orthonormal

basis of $L^2(\Omega, \sigma(\boldsymbol{\theta}), \mathbb{P})$, see e.g. [14]. The random variable $\kappa(\cdot, x) = \exp \gamma(\cdot, x)$ is $\sigma(\boldsymbol{\theta})$ -measurable for almost all $x \in D$ and it holds

$$\mathbb{E}(\kappa(\cdot, x) \frac{1}{\sqrt{\boldsymbol{\nu}!}} H_{\boldsymbol{\nu}}(\boldsymbol{\theta})) = m_{\kappa}(x) \cdot \prod_{k=1}^{\infty} \frac{[\sqrt{\lambda_k} \gamma_k(x)]^{\nu_k}}{\sqrt{\nu_k!}}, \quad (5)$$

see for example [15, p. 71] or [29, p. 16]. Thus the expansion of $\tilde{\kappa} = \kappa - m_{\kappa}$ into the orthonormal basis $\{\frac{1}{\sqrt{\boldsymbol{\nu}!}} H_{\boldsymbol{\nu}}(\boldsymbol{\theta}) \otimes \kappa_{\boldsymbol{\nu}} \mid \boldsymbol{\nu} \in (\mathbb{N}_0)_c^{\mathbb{N}}, \boldsymbol{\nu} \in \mathbb{N}\}$ has the Fourier coefficients

$$\begin{aligned} \xi_{\boldsymbol{\nu}}^{(\boldsymbol{\nu})} &= \frac{1}{\sqrt{\boldsymbol{\nu}!}} \int_D \kappa_{\boldsymbol{\nu}}(x) \cdot \mathbb{E}(\tilde{\kappa}(\cdot, x) H_{\boldsymbol{\nu}}(\boldsymbol{\theta})) dx = \mathbb{E} \left(\xi_{\boldsymbol{\nu}} \cdot \frac{1}{\sqrt{\boldsymbol{\nu}!}} H_{\boldsymbol{\nu}}(\boldsymbol{\theta}) \right) \\ &= \int_D \kappa_{\boldsymbol{\nu}}(x) \cdot m_{\kappa}(x) \cdot \prod_{k=1}^{\infty} \frac{[\sqrt{\lambda_k} \gamma_k(x)]^{\nu_k}}{\sqrt{\nu_k!}} dx - \int_D \kappa_{\boldsymbol{\nu}}(x) m_{\kappa}(x) dx \cdot \delta_{\mathbf{0}, \boldsymbol{\nu}}, \end{aligned} \quad (6)$$

where $\delta_{\mathbf{0}} = \delta_{\nu_1 0} \cdot \delta_{\nu_2 0} \cdots$ is the product of the usual Kronecker deltas.

Let $V_N \subseteq H_0^1(D)$ be an N -dimensional subspace with basis $\{\varphi_1, \dots, \varphi_N\} \subset V_N$. The subspace in $L^2(\Omega)$ will be chosen accordingly to a given number of stochastic variables $K \in \mathbb{N}$ and the maximal degrees of the multivariate Hermite polynomials $\mathbf{p} = (p_1, \dots, p_K) \in \mathbb{N}^K$. The subset $\mathcal{J}_{\mathbf{p}} \subseteq (\mathbb{N})_c^{\mathbb{N}}$ consists of all sequences $\boldsymbol{\alpha} \in (\mathbb{N}_0)_c^{\mathbb{N}}$ such that $0 \leq \alpha_k \leq p_k$ for all $k = 1, \dots, K$ and $\alpha_k = 0$ for all $k > K$. Let $S_{\mathcal{J}_{\mathbf{p}}} \subseteq L^2(\Omega)$ be the subspace spanned by $\{H_{\boldsymbol{\alpha}}(\boldsymbol{\theta}) \mid \boldsymbol{\alpha} \in \mathcal{J}_{\mathbf{p}}\}$.

The bilinear form \mathbf{a} applied to these basis elements of $S_{\mathcal{J}_{\mathbf{p}}} \otimes V_N$ yields (see also [8])

$$\mathbf{a}(H_{\boldsymbol{\alpha}}(\boldsymbol{\theta}) \otimes \varphi_i, H_{\boldsymbol{\beta}}(\boldsymbol{\theta}) \otimes \varphi_j) \quad (7)$$

$$= \int_D m_{\kappa}(x) \nabla \varphi_i(x) \cdot \nabla \varphi_j(x) dx \cdot \delta_{\boldsymbol{\alpha} \boldsymbol{\beta}} \quad (8)$$

$$+ \sum_{l=1}^{\infty} \sum_{\boldsymbol{\nu} \in (\mathbb{N})_c^{\mathbb{N}}} \xi_{\boldsymbol{\nu}}^{(\boldsymbol{\nu})} \cdot \mathbb{E}(H_{\boldsymbol{\nu}}(\boldsymbol{\theta}) H_{\boldsymbol{\alpha}}(\boldsymbol{\theta}) H_{\boldsymbol{\beta}}(\boldsymbol{\theta})) \cdot \int_D \kappa_{\boldsymbol{\nu}}(x) \nabla \varphi_i(x) \cdot \nabla \varphi_j(x) dx \quad (9)$$

$$= (\mathbf{K}_0)_{ij} \cdot (\boldsymbol{\Delta}_0)_{\boldsymbol{\alpha} \boldsymbol{\beta}} + \sum_{l=1}^{\infty} (\mathbf{K}_l)_{ij} \sum_{\boldsymbol{\nu} \in (\mathbb{N}_0)_c^{\mathbb{N}}} \xi_{\boldsymbol{\nu}}^{(\boldsymbol{\nu})} \cdot (\boldsymbol{\Delta}_l)_{\boldsymbol{\alpha} \boldsymbol{\beta}}, \quad (10)$$

wherein

$$(\boldsymbol{\Delta}_l)_{\boldsymbol{\alpha} \boldsymbol{\beta}} = \mathbb{E}(H_{\boldsymbol{\nu}}(\boldsymbol{\theta}) H_{\boldsymbol{\alpha}}(\boldsymbol{\theta}) H_{\boldsymbol{\beta}}(\boldsymbol{\theta})) = \prod_{k=1}^{\infty} \mathbb{E}(h_{\nu_k}(\theta_k) h_{\alpha_k}(\theta_k) h_{\beta_k}(\theta_k)), \quad (11)$$

$$(\mathbf{K}_l)_{ij} = \int_D \kappa_l(x) \nabla \varphi_i(x) \cdot \nabla \varphi_j(x) dx \quad \text{for } l > 0 \text{ and} \quad (12)$$

$$(\mathbf{K}_0)_{ij} = \int_D m_{\kappa}(x) \nabla \varphi_i(x) \cdot \nabla \varphi_j(x) dx. \quad (13)$$

It is worth noting that the summation over $\boldsymbol{\nu}$ can be restricted to $\boldsymbol{\nu} \in \mathcal{J}_{2\mathbf{p}}$, since $(\boldsymbol{\Delta}_{\boldsymbol{\nu}})_{\boldsymbol{\alpha} \boldsymbol{\beta}} := \mathbb{E}(h_{\nu_k}(\theta_k) h_{\alpha_k}(\theta_k) h_{\beta_k}(\theta_k)) = 0$ for $\nu_k > \alpha_k + \beta_k$. By (11), $\boldsymbol{\Delta}_l = \bigotimes_{k=1}^K \boldsymbol{\Delta}_{l_k}$

holds and thus, finally, the stiffness matrix \mathbf{K} can be written as

$$\mathbf{K} = \mathbf{\Delta}_0 \otimes \mathbf{K}_0 + \sum_{l=1}^{\infty} \sum_{\iota \in \mathcal{J}_{2p}} \xi_l^{(\iota)} \cdot \left(\bigotimes_{k=1}^K \mathbf{\Delta}_{\iota_k} \right) \otimes \mathbf{K}_l \in \mathcal{T} := \left(\bigotimes_{k=1}^K \mathbb{R}^{p_k \times p_k} \right) \otimes \mathbb{R}^{N \times N}. \quad (14)$$

As a further step of discretisation we truncate the series in (14) to $M \in \mathbb{N}$ terms. The error measured in the Frobenius norm is bounded by some constant times $\sum_{l=M+1}^{\infty} \lambda_l$, which tends to zero for $M \rightarrow \infty$. In the following we shall simply write \mathbf{K} for the truncated series and $\boldsymbol{\xi}$ for the tensor consisting of all coefficients $\xi_l^{(\iota)}$. It holds $\boldsymbol{\xi} \in \left(\bigotimes_{k=1}^K \mathbb{R}^{p_k} \right) \otimes \mathbb{R}^M$.

The number of entries in the stiffness matrix \mathbf{K} depends exponentially on the number K of random variables $\theta_1, \dots, \theta_K$ used for the stochastic Galerkin discretisation. However, in order to minimize the error of this discretisation it is important to choose the finite dimensional space $\mathcal{S}_{\mathcal{J}_p} \otimes V_N \subseteq L^2(\Omega) \otimes H_0^1(D)$ as large as possible.

The main purpose of this article is to approximate the coefficients tensor $\boldsymbol{\xi}$ in (14) by a tensor $\boldsymbol{\eta} \in \left(\bigotimes_{k=1}^K \mathbb{R}^{p_k} \right) \otimes \mathbb{R}^M$ represented in the canonical tensor format. If $\boldsymbol{\eta}$ is given by $\eta_l^{(\iota)} = \sum_{j=1}^R \prod_{k=1}^K (\eta_{jk})_{\iota_k} \cdot (\eta_j)_l$, we have

$$\begin{aligned} \mathbf{L} &= \mathbf{\Delta}_0 \otimes \mathbf{K}_0 + \sum_{l=1}^M \sum_{\iota \in \mathcal{J}_{2p}} \left[\sum_{j=1}^R \prod_{k=1}^K (\eta_{jk})_{\iota_k} (\eta_j)_l \right] \left(\bigotimes_{k=1}^K \mathbf{\Delta}_{\iota_k} \right) \otimes \mathbf{K}_l \\ &= \mathbf{\Delta}_0 \otimes \mathbf{K}_0 + \sum_{j=1}^R \left(\bigotimes_{k=1}^K \left[\sum_{\iota_k=0}^{2p_k} (\eta_{jk})_{\iota_k} \mathbf{\Delta}_{\iota_k} \right] \right) \otimes \left[\sum_{l=1}^M (\eta_j)_l \mathbf{K}_l \right]. \end{aligned} \quad (15)$$

Obviously, the representation of $\boldsymbol{\eta}$ in the canonical tensor format leads us to a representation of \mathbf{L} in the canonical tensor format in $\left(\bigotimes_{k=1}^K \mathbb{R}^{p_k \times p_k} \right) \otimes \mathbb{R}^{N \times N}$, whose rank is bounded by the representation rank R of $\boldsymbol{\eta}$.

The main advantage of the canonical tensor representation is the linear scaling in K of further numerical operations like matrix-vector multiplication, computation of the maximum (minimum) value and level-sets of the tensor, see e.g. [3, 8, 12] for more details.

Since one is usually interested in a solution u of (1) it is important to estimate the error between the exact solution u and the solution \hat{u} which stems from (1) if we replace the conductivity κ by $\hat{\kappa}$ with a different Fourier coefficients tensor $\boldsymbol{\eta}$ instead of $\boldsymbol{\xi}$.

One possible measure of the impact is the L^p -norm of the relative error, i.e. of the function $\omega \in \Omega \mapsto \|u(\omega, \cdot) - \hat{u}(\omega, \cdot)\|_{H^1(D)} / \|u(\omega, \cdot)\|_{H^1(D)}$. In order to estimate this error we have to make a further assumption.

Assumption 2. It holds $\sum_{k=1}^{\infty} \sqrt{\lambda_k} \|\gamma_k\|_{\infty} < \infty$.

Remark 1.1. This series converges for example, if the covariance function of γ is sufficiently smooth, see [27, Subsections 2.2 and 2.3]. Since the covariance function of γ is determined by the covariance function of κ as seen in (3), the smoothness of Γ_{κ} carries over to Γ_{γ} .

In [10, Lemma 2.5] it is shown, that under the last assumption there exists a positive minimum function $\omega \in \Omega \mapsto \underline{\kappa}(\omega)$ such that it holds $0 < \underline{\kappa} \leq \kappa(\cdot, x)$ \mathbb{P} -almost surely for almost all $x \in D$.

Using $\mathbf{a}(\omega; v, w) := \int_D \kappa(\omega, x) \nabla v(x) \cdot \nabla w(x) dx$ for $u, v \in H^1(D)$ and accordingly $\widehat{\mathbf{a}}$ with $\widehat{\kappa}$ we get

$$\begin{aligned} 0 \leq \underline{\kappa}(\omega) \cdot \|u(\omega, \cdot) - \widehat{u}(\omega, \cdot)\|_{H^1(D)}^2 &\leq \mathbf{a}(\omega; u(\omega, \cdot) - \widehat{u}(\omega, \cdot), u(\omega, \cdot) - \widehat{u}(\omega, \cdot)) \\ &= (\mathbf{a} - \widehat{\mathbf{a}})(\omega; u(\omega, \cdot), u(\omega, \cdot) - \widehat{u}(\omega, \cdot)) \\ &\leq \|\kappa(\omega, \cdot) - \widehat{\kappa}(\omega, \cdot)\|_{L^\infty(D)} \cdot \|u(\omega, \cdot)\|_{H^1(D)} \cdot \|u(\omega, \cdot) - \widehat{u}(\omega, \cdot)\|_{H^1(D)}. \end{aligned}$$

In [10, Lemma 3.10] it is shown that $\mathbb{E}(1/\underline{\kappa}^2) < \infty$ and since that it holds

$$\mathbb{E} \left(\frac{\|u - \widehat{u}\|_{H^1(D)}}{\|u\|_{H^1(D)}} \right)^2 \leq \mathbb{E} \left(\frac{1}{\underline{\kappa}^2} \right) \cdot \mathbb{E}(\|\kappa - \widehat{\kappa}\|_{L^\infty(D)}^2), \quad (16)$$

and with $\|\cdot\|_F$ denoting the Frobenius norm, i.e. $\|\boldsymbol{\xi}\|_F^2 = \sum_{\iota \in \mathcal{J}_{2p}} \sum_{l=1}^M |\xi_l^{(\iota)}|^2$, this yields

$$\mathbb{E}(\|\kappa - \widehat{\kappa}\|_{L^\infty(D)}^2) \leq \sum_{l=1}^M \sum_{\iota \in \mathcal{J}_{2p}} [\xi_l^{(\iota)} - \eta_l^{(\iota)}]^2 \cdot \sum_{l=1}^M \lambda_l \|\kappa_l\|_{L^\infty(D)}^2 \quad (17)$$

$$= \|\boldsymbol{\xi} - \boldsymbol{\eta}\|_F^2 \cdot \sum_{l=1}^M \lambda_l \|\kappa_l\|_{L^\infty(D)}^2. \quad (18)$$

Together with the previous inequalities we conclude, that the L^1 -norm of the relative error $\|u(\omega, \cdot) - \widehat{u}(\omega, \cdot)\|_{H^1(D)} / \|u(\omega, \cdot)\|_{H^1(D)}$ can be made arbitrarily small if $\|\boldsymbol{\xi} - \boldsymbol{\eta}\|_F$ is close enough to zero. Therefore, if we want to approximate $\boldsymbol{\xi}$ by an $\boldsymbol{\eta}$, this has to be done with respect to the Frobenius norm.

Section 2 gives a quick survey of the most common tensor formats along with the most important properties and some remarks on the conversion from the canonical tensor format. Section 3 contains the construction of the approximation $\boldsymbol{\eta}$ of $\boldsymbol{\xi}$ and the main theorem, which essentially states that the introduced error does not depend on the number of random variables K nor the maximal degrees of the multivariate Hermite polynomials \mathbf{p} but on the smoothness of the covariance function Γ_κ . Applying the aforementioned theorem to the Gaussian covariance function on a domain being the union of cuboidal domains, we are led to concrete rank estimates for this case. In Subsection 4.1 we further approximate the tensor approximations obtained by the quadrature method in the canonical tensor format with smaller ranks, in order to assess how conservative the rank estimates of the main theorem are. In Subsection 4.2 we convert the given tensors into the tensor train (TT) and hierarchical tensor formats to test whether those may lead to even better compressions with respect to the storage requirements and complexity of the inner product by an elementary tensor.

2 Tensor formats

Let $\mathcal{V} = \bigotimes_{\nu=1}^K V_\nu$ be the tensor product of vector spaces V_1, \dots, V_K . A tensor format is described by a parameter space $P = \times_{\nu=1}^L P_\nu$ ($K \leq L$) and a multilinear map $U : P \rightarrow \mathcal{V}$ into the tensor space \mathcal{V} . For practical implementations of high dimensional problems we need to distinguish between a tensor $v \in \mathcal{V}$ and its tensor format representation $p \in P$, where $v = U(p)$. There are many possibilities to define tensor formats. Here, we consider the canonical, the hierarchical, and the tensor train format (see [11, 13] and [24, 25]). In the following we briefly repeat the definitions of these formats, for a complete overview see the book of Hackbusch [12]. The last two tensor formats are so called tensor networks, we refer to [6] for a mathematical description of tensor networks.

2.1 The canonical tensor format

Definition 2.1 (Canonical Tensor Format, r-Term Representation, Representation Rank, Representation System). *The canonical tensor format in \mathcal{V} for variable r is defined by the multilinear mapping*

$$U_{CT,r} : P_{CT,r} := \times_{\nu=1}^K V_\nu^r \rightarrow \mathcal{V}, \quad (19)$$

$$p := (p_{i\nu} : 1 \leq i \leq r, 1 \leq \nu \leq K) \mapsto U_{CT,r}(p) := \sum_{i=1}^r \bigotimes_{\nu=1}^K p_{i\nu}.$$

We call the sum of elementary tensors $v = \sum_{i=1}^r \bigotimes_{\nu=1}^K p_{i\nu}$ a tensor represented in the canonical tensor format with r terms. The system of vectors $(p_{i\mu} : 1 \leq i \leq r, 1 \leq \mu \leq d)$ is a representation system of v with representation rank r .

Remark 2.2. Let $v = U_{CT,r}(p) = \sum_{j=1}^r \bigotimes_{\nu=1}^K p_{j\nu}$ be represented in the canonical tensor format with r -terms and representation system $p \in P_{CT,r}$. For the standard choice $V_\nu = \mathbf{R}^{n_\nu}$ the storage size for the parameter system \hat{v} is

$$r \cdot \sum_{\nu=1}^d n_\nu.$$

Numerical operations with tensors represented in the canonical format can be performed linear in K . For instance, let $A = \sum_{l=1}^s \bigotimes_{\nu=1}^K A_{l\nu} \in \bigotimes_{\nu=1}^K \mathbf{R}^{n_\nu \times n_\nu}$ be represented with s -terms then the matrix-vector product of Av is given by

$$Av = \sum_{l=1}^s \sum_{j=1}^r \bigotimes_{\nu=1}^K A_{l\nu} v_{j\nu}.$$

We need $\mathcal{O}\left(r \cdot s \cdot \sum_{\nu=1}^K n_\nu^2\right)$ arithmetic operations to compute a representation system of Av .

A complete description of fundamental operations in the canonical tensor format and a their numerical cost can be found in [12]. For recent algorithms in the canonical tensor format we refer to [3, 4, 5, 8, 9].

2.2 The hierarchical tensor format

The hierarchical tensor format is introduced in [13] and further considered in [11]. Certainly, the hierarchical approach has been discussed earlier in quantum computing (see e.g. [17]). In this section, we briefly repeat the description in [12, 13]. In the following let $\tilde{K} := \{1, \dots, K\}$.

Definition 2.3 (Dimension Partition Tree, [12]). *The tree T_D is called dimension partition tree of \tilde{K} if*

- (1) *all vertices $t \in T_{\tilde{K}}$ are non-empty subsets of \tilde{K} ,*
- (2) *\tilde{K} is the root of $T_{\tilde{K}}$,*
- (3) *every vertex $t \in T_{\tilde{K}}$ with $\#t \geq 2$ has two sons $t_1, t_2 \in T_{\tilde{K}}$ with $t = t_1 \dot{\cup} t_2$.*

The set of sons of t is denoted by $S(t)$. If $S(t) = \emptyset$, t is called a leaf. The set of leaves is denoted by $\mathcal{L}(T_{\tilde{K}})$.

Let $T_{\tilde{K}}$ be a dimension partition tree. The hierarchical tensor representation in $\mathcal{V} = \bigotimes_{\nu \in \tilde{K}} V_\nu$ is based on a hierarchy of finite dimensional tensor product subspaces

$$U_t \subset \mathcal{V}_t := \bigotimes_{\nu \in t} V_\nu \quad \text{for all } t \in T_{\tilde{K}}.$$

Definition 2.4 (Hierarchical Subspace Family, [12]). *We call $\{U_t : t \in T_{\tilde{K}}\}$ a hierarchical subspace family, if $T_{\tilde{K}}$ is a dimension partition tree and the subspaces U_t satisfy*

- (1) *$U_t \subseteq V_t$ for all $t \in \mathcal{L}(T_{\tilde{K}})$,*
- (2) *(crucial nestedness) $U_t \subset U_{t_1} \otimes U_{t_2}$ for all $t \in T_{\tilde{K}} \setminus \mathcal{L}(T_{\tilde{K}})$, $t_1, t_2 \in S(t)$.*

We say a tensor v is represented by the hierarchical subspace family $\{U_t : t \in T_{\tilde{K}}\}$, if $v \in U_{\tilde{K}}$.

The subspace U_t is generated by the system

$$B_t = \left(b_\ell^{(t)} \in U_t : 1 \leq \ell \leq r_t \right), \quad U_t = \text{span} B_t.$$

Except for $t \in \mathcal{L}(T_{\tilde{K}})$, the tensors $b_\ell^{(t)}$ are served for theoretical purpose. Only for leaves, the spanning vectors are explicitly represented. Because of the crucial nestedness

condition, the vectors $b_\ell^{(t)} \in U_t$ ($t \in T_{\tilde{K}} \setminus \mathcal{L}(T_{\tilde{K}})$) can be represented hierarchically by coefficient matrices $C^{(t,\ell)}$, i.e. we have

$$b_\ell^{(t)} = \sum_{i=1}^{r_{t_1}} \sum_{j=1}^{r_{t_2}} C_{ij}^{(t,\ell)} b_i^{(t_1)} \otimes b_j^{(t_2)}, \text{ where } S(t) = \{t_1, t_2\}.$$

The representation of a tensor v represented by the hierarchical subspace family $\{U_t : t \in T_{\tilde{K}}\}$ uses the parameter $C^{(t,\ell)}$ for $t \in T_{\tilde{K}} \setminus \mathcal{L}(T_{\tilde{K}})$ and $b_j^{(t)}$ for $\{t\} \in \mathcal{L}(T_{\tilde{K}})$. Only for theoretical discussion the implicit hierarchical representation of $b_\ell^{(t)}$ for $t \in T_{\tilde{K}} \setminus \mathcal{L}(T_{\tilde{K}})$ is considered. Similarly, to the canonical tensor format, numerical operations with tensors represented in the hierarchical format can be performed linear in K . We refer to [12] for a complete description of the hierarchical format and fundamental operations in this tensor representation.

2.3 The tensor train format

The tensor train (TT) format is described in [24, 25], see also matrix product states (MPS) [30] and references therein.

Definition 2.5 (TT-Format, TT-Representation, TT-Ranks). *The TT-tensor format is for variable TT-representation ranks $\underline{r} = (r_1, \dots, r_{K-1}) \in \mathbb{N}^{K-1}$ defined by the following multilinear mapping*

$$U_{TT} : V_1^{r_1} \times \left(\prod_{\nu=2}^{K-2} V_\nu^{r_{\nu-1} \times r_\nu} \right) \times V_K^{r_{K-1}} \rightarrow \bigotimes_{\nu=1}^K V_\nu \quad (20)$$

$$p = (p_1, \dots, p_K) \mapsto U_{TT}(\hat{v}) := \sum_{j_1=1}^{r_1} \cdots \sum_{j_{K-1}=1}^{r_{K-1}} p_{j_1 1} \otimes \left(\bigotimes_{\nu=2}^{K-2} p_{j_{\nu-1} j_\nu \nu} \right) \otimes p_{j_{K-1} K}.$$

As mentioned for the tensor formats above, the numerical cost for operation with tensors represented in the TT-format is linear in K , see for example [12, 24, 25].

2.4 Conversion from the canonical format

Let a tensor $v = U_{CT}(\hat{v}_{CT}) = \sum_{j=1}^r \bigotimes_{\nu=1}^K v_{j\nu}$ be represented in the canonical tensor format with representation system $\hat{v}_{CT} \in P_{TC,r}$. We discuss the simple conversion of v into the hierarchical tensor format and the TT-format, i.e. we define representation systems $\hat{u}_{\mathcal{H}} \in P_{\mathcal{H},\underline{r}}$ and $\hat{u}_{TT} \in P_{TT,\underline{r}}$ such that

$$v = U_{\mathcal{H}}(\hat{v}_{\mathcal{H}}) = U_{TT}(\hat{v}_{TT}).$$

Remark 2.6 (Conversion to the hierarchical tensor representation). *Let $v \in \text{range } U_{CT,r}$ be represented in the canonical tensor format with r -terms, e.g. $v = \sum_{j=1}^r \bigotimes_{\nu=1}^K v_{j\nu}$.*

Let $T_{\tilde{K}}$ be a dimension partition tree for $\tilde{K} := \{1, \dots, K\}$. The hierarchical subspace family $\{U_t : t \in T_{\tilde{K}}\}$ is generated by the the systems

$$B_t = \left(b_j^{(t)} \in U_t : 1 \leq j \leq r \right), \quad U_t = \text{span} B_t,$$

where

$$b_j^{(t)} := \bigotimes_{\nu \in t} v_{j\nu}, \quad \text{for } t \in T_{\tilde{K}} \setminus \tilde{K}.$$

Since $b_j^{(t)} = b_j^{(t_1)} \otimes b_j^{(t_2)}$, the coefficient matrices have for $t \in T_{\tilde{K}} \setminus \tilde{K}$ the form

$$c_{ij}^{t,\ell} := \delta_{ij} \delta_{j\ell}, \quad (1 \leq i, j, \ell \leq r)$$

where $S(t) = \{t_1, t_2\}$. For $t = \tilde{K}$ the coefficient matrix $C^{\tilde{K},1}$ is equal to \mathbf{Id} , see [12].

Remark 2.7 (Conversion to the TT-tensor representation). Let $v = \sum_{j=1}^r \bigotimes_{\nu=1}^K v_{j\nu} \in \text{range } U_{CT}$. Then define $\underline{r} := (r, \dots, r) \in \mathbb{N}^{K-1}$ and for $1 \leq j_1, \dots, j_{K-1} \leq r$

$$u_{j_1 1} := v_{j_1 1}, \quad u_{j_{K-1} K} := v_{j_{K-1} K}, \quad u_{j_{\nu-1} j_\nu \nu} := \delta_{j_{\nu-1}, j_\nu} v_{j_\nu \nu} \quad (2 \leq \nu \leq K-1), \quad (21)$$

where δ is Kronecker's delta. With (21) we have that

$$\sum_{j_1=1}^r \cdots \sum_{j_{K-1}=1}^r u_{1j_1} \otimes \bigotimes_{\nu=2}^{K-2} u_{\nu j_{\nu-1} j_\nu} \otimes u_{K j_{K-1}} = \sum_{j=1}^r \bigotimes_{\nu=1}^K v_{j\nu}.$$

3 Low rank approximation of ξ

3.1 Error estimation

The most obvious way to approximate the coefficients tensors ξ from (6) is to apply a quadrature rule to the integral. Since the integrand of ξ already separates we immediately obtain an approximation of ξ in the canonical tensor format. Theorem 3.1 reveals that the error introduced by this approximation does not depend on the number of random variables K nor the maximal degrees of the multivariate Hermite polynomials \mathbf{p} . Nevertheless it depends on the analytical properties of the covariance function Γ_κ and the eigenvalues of the covariance operator \mathcal{C}_κ and the quality of the used quadrature and its error estimation.

Let $C(D)$ the set of continuous functions on D and $\mathcal{Q} : C(D) \rightarrow \mathbb{R}$ a quadrature rule on D with nodes $x_1, \dots, x_R \in D$ and weights $w_1, \dots, w_R \in \mathbb{R}$. Let $\mathcal{E} : C(D) \rightarrow \mathbb{R}$ be the error functional of the quadrature \mathcal{Q} , i.e.

$$\mathcal{E}(f) = \int_D f(x) dx - \mathcal{Q}(f) \in \mathbb{R} \quad (22)$$

for all $f \in C(D)$. In order to approximate the tensor

$$\xi_l^{(\iota)} = \int_D \kappa_l(x) \cdot m_\kappa(x) \cdot \prod_{k=1}^{\infty} \frac{[\sqrt{\lambda_k} \gamma_k(x)]^{\iota_k}}{\sqrt{\iota_k!}} dx - \int_D \kappa_l(x) m_\kappa(x) dx \cdot \delta_{0\iota} \quad (23)$$

by a tensor $\boldsymbol{\eta} = (\eta_l^{(\boldsymbol{\iota})})_{l \in \{1, \dots, M\}, \boldsymbol{\iota} \in \mathcal{J}_{2p}} \in \left(\bigotimes_{k=1}^K \mathbb{R}^{p_k} \right) \otimes \mathbb{R}^M$, we apply the quadrature rule \mathcal{Q} and get

$$\eta_l^{(\boldsymbol{\iota})} = \mathcal{Q} \left(\kappa_l \cdot m_\kappa \cdot \prod_{k=1}^K \frac{[\sqrt{\lambda_k} \gamma_k]^{\iota_k}}{\iota_k!} \right) - \mathcal{Q}(\kappa_l m_\kappa) \cdot \delta_{0\boldsymbol{\iota}} \quad (24)$$

$$= \sum_{j=1}^R w_j \kappa_l(x_j) m_\kappa(x_j) \prod_{k=1}^K \frac{[\sqrt{\lambda_k} \gamma_k(x_j)]^{\iota_k}}{\iota_k!} - \left(\sum_{j=1}^R w_j \kappa_l(x_j) m_\kappa(x_j) \right) \cdot \delta_{0\boldsymbol{\iota}}. \quad (25)$$

Theorem 3.1. *The rank of $\boldsymbol{\eta}$ defined in (24) is bounded by $R+1$, where R is the number of quadrature nodes. It holds*

$$\|\boldsymbol{\xi} - \boldsymbol{\eta}\|_F^2 \leq (\mathcal{E} \otimes \mathcal{E}) \left(\left[\sum_{l=1}^M \kappa_l \otimes \kappa_l \right] \cdot \Gamma_\kappa \right), \quad (26)$$

where Γ_κ is the covariance function of the random field κ and $\kappa_1, \dots, \kappa_M$ the first M eigenfunctions of the associated covariance operator.

The error between $\boldsymbol{\xi}$ and $\boldsymbol{\eta}$ does not depend on the number of stochastic variables K nor on the maximal degrees of the multivariate Hermite polynomials \mathbf{p} .

The functional $\mathcal{E} \otimes \mathcal{E} : C(D) \otimes C(D) \rightarrow \mathbb{R}$ denotes the tensor product functional, i.e. $(\mathcal{E} \otimes \mathcal{E})(f \otimes g) = \mathcal{E}(f) \cdot \mathcal{E}(g)$ for all $f, g \in C(D)$. The value of the function $h \in C(D \times D) = C(D) \otimes C(D)$ applied to this functional can be seen as the consecutively application of \mathcal{E} to the first argument and then to the second one or vice versa.

Proof. The representation of $\boldsymbol{\eta}$ in the canonical tensor format in (24) has a representation rank $R+1$. Furthermore it holds

$$\sum_{\boldsymbol{\iota} \in (\mathbb{N}_0)^N} \frac{1}{\boldsymbol{\iota}!^2} \mathbb{E}[\tilde{\kappa}(\cdot, x) H_{\boldsymbol{\iota}}(\boldsymbol{\theta})] \mathbb{E}[\tilde{\kappa}(\cdot, y) H_{\boldsymbol{\iota}}(\boldsymbol{\theta})] = \mathbb{E}[\tilde{\kappa}(\cdot, x) \tilde{\kappa}(\cdot, y)] = \Gamma_\kappa(x, y), \quad (27)$$

since the Hermite polynomials form an orthogonal basis of $L^2(\Omega, \sigma(\boldsymbol{\theta}))$. For $l \in \{1, \dots, M\}$

we thus get

$$\sum_{\iota \in \mathcal{J}_{2p}} |\xi_l^{(\iota)} - \eta_l^{(\iota)}|^2 \quad (28)$$

$$= \sum_{\iota \in \mathcal{J}_{2p}} \left[\int_D \int_D \frac{1}{\iota!^2} \kappa_l(x) \kappa_l(y) \mathbb{E}(\tilde{\kappa}(\cdot, x) H_\iota(\boldsymbol{\theta})) \mathbb{E}(\tilde{\kappa}(\cdot, x) H_\iota(\boldsymbol{\theta})) dx dy \quad (29)$$

$$- 2 \int_D \sum_{j=1}^R w_j \frac{1}{\iota!^2} \kappa_l(x) \kappa_l(x_j) \mathbb{E}(\tilde{\kappa}(\cdot, x) H_\iota(\boldsymbol{\theta})) \mathbb{E}(\tilde{\kappa}(\cdot, x_j) H_\iota(\boldsymbol{\theta})) dy \quad (30)$$

$$+ \sum_{i=1}^R \sum_{j=1}^R w_i w_j \frac{1}{\iota!^2} \kappa_l(x_i) \kappa_l(x_j) \mathbb{E}(\tilde{\kappa}(\cdot, x_i) H_\iota(\boldsymbol{\theta})) \mathbb{E}(\tilde{\kappa}(\cdot, x_j) H_\iota(\boldsymbol{\theta})) \Big] \quad (31)$$

$$\leq \sum_{\iota \in (\mathbb{N}_0)^{\mathbb{N}_c}} [\dots] \quad (32)$$

$$= \int_D \int_D \kappa_l(x) \kappa_l(y) \Gamma_\kappa(x, y) dx dy - 2 \int_D \sum_{j=1}^R w_j \kappa_l(x) \kappa_l(x_j) \Gamma_\kappa(x, x_j) dx \quad (33)$$

$$+ \sum_{i=1}^R \sum_{j=1}^R w_i w_j \kappa_l(x_i) \kappa_l(x_j) \Gamma_\kappa(x_i, x_j) \quad (34)$$

$$= (\mathcal{E} \otimes \mathcal{E})([\kappa_l \otimes \kappa_l] \cdot \Gamma_\kappa) \quad (35)$$

Finally, summation over all l yields (26). \blacksquare

Remark 3.2. 1. *Even though the accuracy of the approximation $\boldsymbol{\eta}$ does not depend on the number of random variables nor the maximal degrees of the multivariate Hermite polynomials \mathbf{p} , the amount of data to be stored is still $(R+1) \cdot \sum_{k=1}^K p_k$, depends on K and \mathbf{p} .*

2. *A smoother covariance function with smoother eigenfunctions permits better quadrature methods \mathcal{Q} , i.e. those with fewer nodes and sharper estimates of $|(\mathcal{E} \otimes \mathcal{E})(f)|$. Thus the representation rank of the approximation to a given accuracy depends on the smoothness of the covariance function.*

3. *If there exists $n \in \mathbb{N}$ such that the derivatives $\partial_x^i \partial_y^j \Gamma_\kappa$ for $i, j \leq n$ exist and are continuous, the random field κ must be n -times mean-square differentiable (see [1, Theorem 2.2.2].) Thus more rough random fields κ will lead to larger ranks of the approximation $\boldsymbol{\eta}$.*

3.2 Gaussian covariance on cuboidal domains

Let $D = \bigcup_{m=1}^L C_m$, where $C_1, \dots, C_L \subset \mathbb{R}^d$ are closed cuboidal domains, whose pairwise intersections are sets of measure zero in \mathbb{R}^d . For a given $a > 0$, we set $\Gamma_\kappa(x, y) = \exp(-a^2 \|x - y\|^2)$ for all $x, y \in D$. The value $\frac{1}{a}$ characterizes the covariance length.

Theorem 3.3. *Let \mathcal{Q} denote the compound quadrature rule, which consists of d -fold product quadratures of S -point Gaussian quadratures on each cuboidal domain C_m . Let $\boldsymbol{\eta}$ be the approximation of $\boldsymbol{\xi}$ as defined in (24), then $\boldsymbol{\eta}$ has the representation rank $S^d L$ with the norm estimation*

$$\begin{aligned} \|\boldsymbol{\eta} - \boldsymbol{\xi}\|_F^2 &\leq \sum_{l=1}^M \mathcal{E} \otimes \mathcal{E}(\kappa_l \otimes \kappa_l \Gamma_\kappa) \\ &\leq \sum_{l=1}^M \frac{1}{\lambda_l^2} \cdot \frac{a^{4S} |D|}{(2S)!} \sum_{m=1}^L \sum_{n=1}^L |C_m| |C_n| \sum_{i=1}^d \sum_{j=1}^d \text{diam}_i(C_m)^{2S} \text{diam}_j(C_n)^{2S} \\ &\quad \cdot \exp\left[\frac{1}{4}a^2 \text{diam}_i(D) + \frac{1}{4}a^2 \text{diam}_j(D)\right] \left[1 + \left(\left(\frac{3}{2}\right)^{2S} - 1\right)\delta_{ij}\right]. \end{aligned} \quad (36)$$

Proof. Combining the errors of the quadratures on each cuboidal domain, we get

$$\mathcal{E}(f) = \frac{c_S}{(2S)!} \sum_{m=1}^L |C_m| \sum_{i=1}^d \text{diam}_i(C_m)^{2S} \partial_i^{2S} f(\xi_{im}), \quad (37)$$

where $\xi_{im} \in C_m$, $0 < c_S < 1$, and $f \in C^{2S}(D)$. $\text{diam}_i(A) := \sup\{|x_i - y_i| \mid x, y \in A\}$ denotes the diameter of $A \in \mathbb{R}^d$ in the i -th direction.

Since the Gaussian covariance is sufficiently smooth, this quadrature error can be applied and we have to estimate

$$\begin{aligned} \|\boldsymbol{\xi} - \boldsymbol{\eta}\|_F^2 &\leq \sum_{l=1}^M \mathcal{E} \otimes \mathcal{E}(\kappa_l \otimes \kappa_l \Gamma_\kappa) = \frac{c_S^2}{(2S)!^2} \sum_{m=1}^L \sum_{n=1}^L |C_m| |C_n| \\ &\quad \cdot \sum_{i=1}^d \sum_{j=1}^d \text{diam}_i(C_m)^{2S} \text{diam}_j(C_n)^{2S} \cdot \sum_{l=1}^M \partial_{x_i}^{2S} \partial_{y_j}^{2S} [\kappa_l \otimes \kappa_l \Gamma_\kappa] \Big|_{(\xi_{ijmn}, \eta_{ijmn})}, \end{aligned} \quad (38)$$

where $\xi_{ijmn}, \eta_{ijmn} \in D$. It is

$$\left| \partial_{x_i}^{2S} \partial_{y_j}^{2S} [\kappa_l(x) \kappa_l(y) \Gamma_\kappa(x, y)] \right| \quad (39)$$

$$\leq \frac{1}{\lambda_l^2} \int_D \int_D \left| \partial_{x_i}^{2S} \partial_{y_j}^{2S} [\Gamma_\kappa(x, u) \Gamma_\kappa(y, v) \Gamma_\kappa(x, y)] \kappa_l(u) \kappa_l(v) \right| dudv \quad (40)$$

$$\leq \frac{1}{\lambda_l^2} \sqrt{\int_D \int_D \left| \partial_{x_i}^{2S} \partial_{y_j}^{2S} [\Gamma_\kappa(x, u) \Gamma_\kappa(y, v) \Gamma_\kappa(x, y)] \right|^2 dudv}, \quad (41)$$

since the eigenfunction κ_l is normalized in $L^2(D)$. For $i = j$ it holds

$$\begin{aligned} \partial_{x_i}^{2S} \partial_{y_i}^{2S} [\Gamma_\kappa(x, u) \Gamma_\kappa(y, v) \Gamma_\kappa(x, y)] &= \Gamma_\kappa(x, u) \Gamma_\kappa(y, v) \Gamma_\kappa(x, y) \cdot \\ &\quad \cdot a^{4S} \sum_{q=0}^{2S} \binom{2S}{q} \frac{(2S)!}{2^{2S-q} q!} h_q\left(ax_i - \frac{a}{2}(y_i + u_i)\right) h_q\left(ay_i - \frac{a}{2}(x_i + v_i)\right). \end{aligned} \quad (42)$$

Cramér's inequality [26, p. 208] guarantees that $|h_q(x)| \leq 1.09\sqrt{q!} \exp(\frac{1}{4}x^2)$ and thus we get

$$\left| \partial_{x_i}^{2S} \partial_{y_i}^{2S} [\Gamma_\kappa(x, u) \Gamma_\kappa(y, v) \Gamma_\kappa(x, y)] \right| \leq (1.09)^2 (\frac{3}{2}a)^{4S} (2S)! \exp[\frac{1}{2}a^2 \text{diam}_i(D)^2]. \quad (43)$$

Accordingly, for $i \neq j$ we get

$$\partial_{x_i}^{2S} \partial_{y_j}^{2S} [\Gamma_\kappa(x, u) \Gamma_\kappa(y, v) \Gamma_\kappa(x, y)] \quad (44)$$

$$= \Gamma_\kappa(x, u) \Gamma_\kappa(y, v) \Gamma_\kappa(x, y) a^{4S} h_{2S}(ax_i - \frac{a}{2}(y_i + u_i)) h_{2S}(ay_j - \frac{a}{2}(x_j + v_j)), \quad (45)$$

and this leads to

$$\left| \partial_{x_i}^{2S} \partial_{y_j}^{2S} [\Gamma_\kappa(x, u) \Gamma_\kappa(y, v) \Gamma_\kappa(x, y)] \right| \leq (1.09)^2 a^{4S} (2S)! \exp[\frac{1}{4}a^2 \text{diam}_i(D) + \frac{1}{4}a^2 \text{diam}_j(D)]. \quad (46)$$

Together these two cases applied to (39) and finally to (38) lead to the asserted inequality (36). \blacksquare

Corollary 3.4. *Let $D = [0, 1]^d \subset \mathbb{R}^d$ be the unit square. The approximation $\boldsymbol{\eta}$ has a tensor rank bounded by $R + 1$ and allows the error estimate*

$$\|\boldsymbol{\eta} - \boldsymbol{\xi}\|_F^2 \leq \sum_{l=1}^M (\mathcal{E} \otimes \mathcal{E})([\kappa_l \otimes \kappa_l] \Gamma_\kappa) \leq \frac{a^{4S} d((d-1) + (\frac{3}{2})^{2S}) \exp(\frac{1}{2}a^2)}{(2S)!} \cdot \sum_{l=1}^M \frac{1}{\lambda_l^2}, \quad (47)$$

where $R = S^d$. Further with $S \geq \frac{3}{4}(ae)^2$ and

$$S > \frac{1}{2} \log \left[d^2 \sum_{l=1}^M \frac{1}{\lambda_l^2} \right] + \frac{a^2}{4} - \frac{1}{4} \log(3\pi a^2) - \log \varepsilon - 1, \quad (48)$$

Stirling's approximation shows, that the error (47) is less than ε .

Table 1 presents the necessary representation ranks of $\boldsymbol{\eta}$ in order to approximate $\boldsymbol{\xi}$ to a relative accuracy of 10^{-6} depending on the dimension of the unit cube D and the Karhunen-Loève truncation parameter M of κ .

Remark 3.5. 1. *For higher dimensions d of the domain D , a more sophisticated quadrature method than the d -fold product quadrature of Gaussian quadratures must be chosen in order to overcome the exponential dependency of R on d . This method however must provide an adequate representation of the error functional \mathcal{E} in order to allow the analysis of the approximation error (26).*

2. *Since the eigenvalues decrease exponentially (cf. [27, Proposition 2.18]), (47) reveals a crucial dependency on the Karhunen-Loève-truncation parameter M . A better knowledge of the behaviour of the eigenfunctions κ_l would lead to a stricter control over the error by superseding estimates like (39).*

a	M	K	p	S	R	$\frac{\ \boldsymbol{\eta}\ _F - \ \kappa\ }{\ \kappa\ }$
1	10	20	10	13	196 (31)	$1.027 \cdot 10^{-4}$
1/2	20	20	10	19	400 (63)	$1.988 \cdot 10^{-4}$
1/3	50	20	10	31	1024 (81)	$13.427 \cdot 10^{-4}$

(a) $D = [0, 1]^2$

a	M	K	p	S	R	$\frac{\ \boldsymbol{\eta}\ _F - \ \kappa\ }{\ \kappa\ }$
1	5	20	10	12	12 (8)	$2.868 \cdot 10^{-6}$
1/2	5	20	10	19	19 (14)	$2.512 \cdot 10^{-5}$
1/3	7	20	10	32	32 (17)	$6.357 \cdot 10^{-4}$
1/4	10	20	10	51	51 (21)	$3.158 \cdot 10^{-4}$

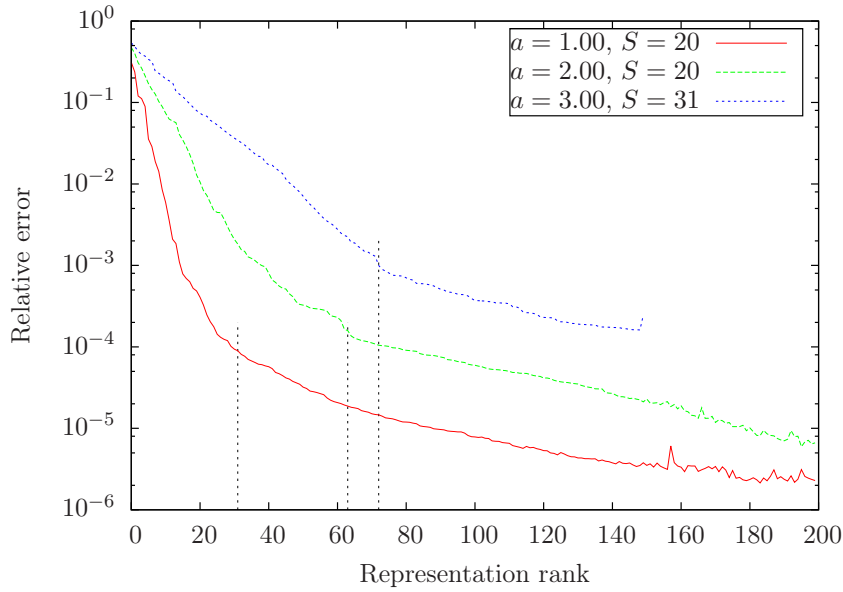
(b) $D = [0, 1]^1$

Table 1: Number of nodes S depending on the given correlation length a in order to achieve a relative error less than 10^{-4} . M denotes the Karhunen-Loève truncation parameter, K the number of random variables, and p the maximal degree of the multivariate Hermite polynomials. S is the number of quadrature nodes of the Gaussian quadrature and R the representation rank of the approximation. The values in the brackets are the suspected canonical tensor rank found by the recompression of $\boldsymbol{\eta}$ with a relative error of at most 10^{-4} .

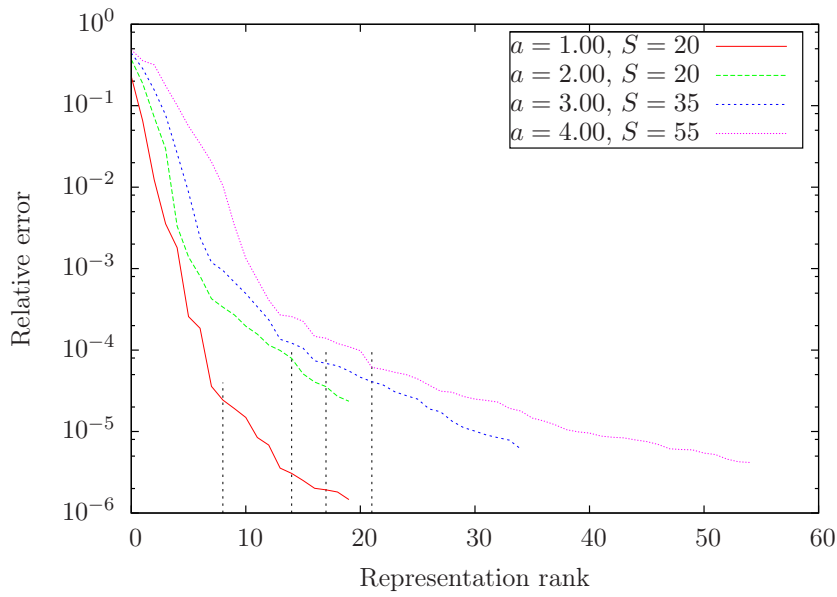
4 Numerical experiences

4.1 Recompression of the $\boldsymbol{\eta}$

In order to test how conservative the obtained approximations $\boldsymbol{\eta}$ are, we approximate them in a low rank representation, i.e. perform a recompression. The general setup is the following: The eigenvalues and eigenfunctions of the covariance operator of κ and γ are approximated as described in [15, Chapter 3]. The used mesh consists in the one-dimensional case of 1001 points and in the two-dimensional case of 2113 points and 4096 triangles. The number of random variables K is fixed to 20 and the maximal degrees of the multivariate Hermite polynomials to $\boldsymbol{p} = (10, \dots, 10, 0, \dots)$. The Karhunen-Loève truncation parameter M is chosen accordingly, in order to obtain a relative error of at most 10^{-4} for the truncated Karhunen-Loève expansion. The approximations $\boldsymbol{\eta}$ obtained by the Gaussian quadrature are approximated in the canonical tensor format with small ranks, in order to estimate the real tensor ranks of $\boldsymbol{\xi}$. The ALS method (see e.g. [12] or [7]) provides an effective and easy to implement method for this purpose. The relative difference between $\|\kappa\|_{L^2(\Omega \times D)}$ and $\|\boldsymbol{\eta}\|_F$ is a lower bound of the overall error. Usually this lower bound can be observed in the low-rank approximation as a threshold, where the ratio between gained error reduction to the rank increase diminishes. In the Figures 1 we see the relative error between the best approximation in the canonical tensor format as a function of the representation rank. A dashed line marks the representation rank reaching the error bound of 10^{-4} . Clearly, the ranks obtained



(a) $D = [0, 1]^2$



(b) $D = [0, 1]^1$

Figure 1: Relative error between η and its recompression with a given representation rank.

by the quadrature approximation are usually too high, especially in the two-dimensional case. As Remark 3.5, already mentioned a more sophisticated quadrature method than the product quadrature of two Gaussian quadratures might lead to better ranks.

4.2 Comparison with other tensor formats

Different tensor formats have different storage requirement and complexities for operations like inner products or point-wise evaluations (cf. [12]). Nevertheless even more complex formats than the canonical format can lead to a significant reduction of the involved ranks and thus to a much better performance. In order to test this possibility, we approximate the canonical tensor obtained by the quadrature method in the TT and the hierarchical tensor format. The TT approximation is accomplished by the TT-Toolbox 2.2 (see [23]), the approximation in hierarchical format by the Hierarchical Tucker Toolbox (see [28]). In both cases the given canonical tensor has to be approximated with a relative accuracy of 10^{-4} , just as the low-rank approximation in the canonical tensor format. In order to compare the different approximations we computed the storage requirements as well as the complexity of the scalar product $\langle \mathbf{L}\mathbf{v}, \mathbf{v} \rangle$ as an overall complexity measure. The matrix \mathbf{L} denotes the approximation of the stiffness matrix \mathbf{K}

$$\mathbf{L} = \sum_{l=1}^M \sum_{\iota \in \mathcal{J}_{2p}} \tilde{\xi}_l^{(\iota)} \cdot \left(\bigotimes_{k=1}^K \Delta_{\iota_k} \right) \otimes \mathbf{K}_l,$$

where $\tilde{\xi}$ is the approximation in the according tensor format and $\mathbf{v} = v_0 \otimes v_1 \otimes \cdots \otimes v_K$ an elementary tensor. Since

$$\langle \mathbf{L}\mathbf{v}, \mathbf{v} \rangle = \sum_{l=1}^M \sum_{\iota \in \mathcal{J}_{2p}} \tilde{\xi}_l^{(\iota)} \cdot \prod_{k=1}^K \langle \Delta_{\iota_k} v_k, v_k \rangle \cdot \langle \mathbf{K}_l v_0, v_0 \rangle, \quad (49)$$

the complexity of this operation corresponds to the scalar product of the approximation $\tilde{\xi}$ with an elementary tensor. Table 2 gathers the obtained results.

Obviously with decreasing covariance length the approximations in the canonical tensor format always outperforms the other formats, since the ranks couldn't be reduced as much as needed. Since that an approximation in the other different formats only seems advantageous if the time needed to calculate the compression is an important factor.

5 Conclusion

We saw that the stochastic Galerkin discretization of the stationary diffusion equation leads to a high dimensional Galerkin matrix whose number of entries depends exponentially on the number of random variables K . In order to overcome this problem we proposed a data sparse representation of this matrix which naturally emerges if we approximate the tensor ξ by an η given the canonical tensor format. The amount of data to be stored as well as the complexity of matrix-vector multiplications decreases

a	CP		TT		HT	
	Storage	$\langle \mathbf{L}\mathbf{v}, \mathbf{v} \rangle$	Storage	$\langle \mathbf{L}\mathbf{v}, \mathbf{v} \rangle$	Storage	$\langle \mathbf{L}\mathbf{v}, \mathbf{v} \rangle$
1	1,640	3,279	905	1,721	637	1,317
1/2	2,870	5,739	1,585	3,013	1,242	2,622
1/3	3,519	7,037	3,425	6,509	1,937	4,113
1/4	4,410	8,819	10,430	19,826	7,024	14,829

(a) $D = [0, 1]^1$

a	CP		TT		HT	
	Storage	$\langle \mathbf{L}\mathbf{v}, \mathbf{v} \rangle$	Storage	$\langle \mathbf{L}\mathbf{v}, \mathbf{v} \rangle$	Storage	$\langle \mathbf{L}\mathbf{v}, \mathbf{v} \rangle$
1	6,510	13,019	15,570	29,592	9,826	20,627
1/2	13,860	27,719	155,310	295,128	148,252	303,673
1/3	20,250	40,499	458,210	870,848	490,780	999,616

(b) $D = [0, 1]^2$

Table 2: Storage requirements and number of arithmetic operations of the given scalar product in the different tensor formats.

dramatically and only depends linearly on the degrees of polynomial chaos p_1, \dots, p_K and polynomial on the representation rank of $\boldsymbol{\eta}$.

Yet Theorem 3.1 pointed out that the rank necessary in order to achieve a given accuracy does not depend on the number of random variables nor on the degrees of polynomial chaos. However it remains a dependency on the Karhunen-Loève-truncation parameter M and the analytic properties of the covariance function Γ_κ and the eigenfunctions $\kappa_1, \kappa_2, \dots$ and eigenvalues $\lambda_1, \lambda_2, \dots$ of its associated integral operator. Theorem 3.3 revealed that this remaining dependency still can get crucial if the eigenfunctions are not known in more detail.

Although the applied product quadrature rule leads to serious issues if the dimensions of domain D gets larger than two, it allowed us an immediate analysis of the error term. In order to get better representation ranks it is necessary to further reduce the number of quadrature points by using more sophisticated quadrature rules. However the right-hand side of (26) makes very rigorous demands on the error estimator \mathcal{E} : It has to be applicable twice on a function with respect to different variables.

Since the given representation ranks are only upper bounds of the algebraic tensor rank of $\boldsymbol{\xi}$, much smaller representation ranks than those obtained by the quadrature rule may be possible. The applied post compression in Subsection 4.1 in the canonical tensor format underlined this. The actually needed ranks for an approximations with a relative error of 10^{-4} are usually only a small fraction of the initial ranks. Nevertheless an approximation in different formats like the TT or the hierarchical tensor format only seems advantageous if the time needed to calculate the compression is an important factor.

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References

- [1] R. J. Adler. *The Geometry of Random Fields*. Wiley, Chichester, New York, Brisbane, 2002.
- [2] I. Babuška, R. Tempone, and G. E. Zouraris. Galerkin finite element approximations of stochastic elliptic partial differential equations. *SIAM J. Numer. Anal.*, 42(2):800–825, 2004.
- [3] M. Espig. *Effiziente Bestapproximation mittels Summen von Elementartensoren in hohen Dimensionen*. PhD thesis, Universität Leipzig, 2008.
- [4] M. Espig, L. Grasedyck, and W. Hackbusch. Black box low tensor rank approximation using fibre-crosses. *Constructive approximation*, 2009.
- [5] M. Espig and W. Hackbusch. A regularized newton method for the efficient approximation of tensors represented in the canonical tensor format. *Num. Math.*, 2012.
- [6] M. Espig, W. Hackbusch, S. Handschuh, and R. Schneider. Optimization problems in contracted tensor networks. *MIS-MPI Preprint 66*, 2011.
- [7] M. Espig, W. Hackbusch, and A. Khachatryan. On the convergence of alternating least squares optimisation in tensor format representations. 2012. To appear 2012.
- [8] M. Espig, W. Hackbusch, A. Litvinenko, H. G. Matthies, and E. Zander. Efficient analysis of high dimensional data in tensor formats. volume 88. LNCSE, 2012.
- [9] M. Espig, W. Hackbusch, T. Rohwedder, and R. Schneider. Variational calculus with sums of elementary tensors of fixed rank. *Numerische Mathematik*, 2012.
- [10] C. J. Gittelsohn. Stochastic galerkin discretization of the log-normal isotropic diffusion problem. *Mathematical Models and Methods in Applied Sciences*, 20(2):237–263, 2010.
- [11] L. Grasedyck. Hierarchical singular value decomposition of tensors. *SIAM J. Matrix Analysis Applications*, 31(4):2029–2054, 2010.
- [12] W. Hackbusch. *Tensor Spaces and Numerical Tensor Calculus*. Springer, 2012. to be published.
- [13] W. Hackbusch and S. Kühn. A new scheme for the tensor representation. *The journal of Fourier analysis and applications*, 5(15):706–722, 2009.
- [14] S. Janson. *Gaussian Hilbert spaces*. Cambridge University Press, 1997.

- [15] A. Keese. *Numerical Solution of Systems with Stochastic Uncertainties*. PhD thesis, Technische Universität Braunschweig, 2004.
- [16] A. Litvinenko and H. G. Matthies. Sparse data representation of random fields. *Proceedings in Applied Mathematics and Mechanics, PAMM Vol. 9, Wiley-InterScience*, pages 587 – 588, 2009.
- [17] C. Lubich. *From quantum to classical molecular dynamics: reduced models and numerical analysis*. Zurich lectures in advanced mathematics. EMS, 2008.
- [18] H. G. Matthies. Uncertainty quantification with stochastic finite elements. 2007. Part 1. Fundamentals. *Encyclopedia of Computational Mechanics*, John Wiley and Sons, Ltd.
- [19] H. G. Matthies and A. Keese. Galerkin methods for linear and nonlinear elliptic stochastic partial differential equations. *Comput. Methods Appl. Mech. Engrg.*, 194(12-16):1295–1331, 2005.
- [20] H. G. Matthies and A. Keese. Galerkin methods for linear and nonlinear elliptic stochastic partial differential equations. *Comput. Methods Appl. Mech. Engrg.*, 194(12-16):1295–1331, 2005.
- [21] H. G. Matthies and E. Zander. Solving stochastic systems with low-rank tensor compression. *Linear Algebra and its Applications*, 436(10):3819 – 3838, 2012.
- [22] A. Mugler and H. J. Starkloff. On elliptic partial differential equations with random coefficients. *Studia Universitatis Babeş-Bolyai Mathematica*, 56(2):473–487, 2011.
- [23] I. Oseledets. TT-Toolbox 2.2. <http://spring.inm.ras.ru/osel/download/tt22.zip>.
- [24] I. V. Oseledets. Tensor-train decomposition. *SIAM J. Scientific Computing*, 33(5):2295–2317, 2011.
- [25] I. V. Oseledets and E. Tyrtyshnikov. Breaking the curse of dimensionality, or how to use SVD in many dimensions. *SIAM J. Scientific Computing*, 31(5):3744–3759, 2009.
- [26] Bateman Manuscript Project, H. Bateman, A. Erdélyi, and United States. Office of Naval Research. *Higher transcendental functions*. Number Bd. 2 in Higher Transcendental Functions. McGraw-Hill, 1953.
- [27] Ch. Schwab and R. A. Todor. Karhunen-Loève approximation of random fields by generalized fast multipole methods. *J. Comput. Phys.*, 217(1):100–122, 2006.
- [28] Ch. Tobler and D. Kressner. Hierarchical tucker toolbox. http://www.sam.math.ethz.ch/NLAGroup/htucker_toolbox.html.

- [29] E. Ullmann. *Solution Strategies for Stochastic Finite Element Discretizations*. PhD thesis, Technische Universität Bergakademie Freiberg, 2008.
- [30] G. Vidal. Efficient classical simulation of slightly entangled quantum computations. *Phys. Rev. Lett.*, 91(14), 2003.

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