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Abstract

We consider a class of multilevel matrices, which arise from the discretization of linear diffusion operators in a d-dimensional hypercube. Under certain assumptions on the structure of the diffusion tensor (motivated by financial models), we derive an explicit representation of such a matrix in the recently introduced *Tensor Train (TT)* format with the *TT ranks* bounded from above by $2 + \left\lfloor \frac{d}{2} \right\rfloor$. We also show that if the diffusion tensor is constant and *semiseparable of order* $r < \left\lfloor \frac{d}{2} \right\rfloor$, the representation can be refined and the bound on the *TT ranks* can be sharpened to $2+r$ (we do this in a more general setting, for non-constant diffusion tensors of a certain structure). As a result, when n degrees of freedom are used in each dimension, such a matrix is represented in the TT format through $\mathcal{O}\left(d^3 n^2\right)$ and $\mathcal{O}\left(d\, n^2 r^2\right)$ parameters resp. instead of its n^{2d} entries. We also discuss the representation of such a matrix in the *Quantized Tensor Train (QTT)* decomposition in terms of $\mathcal{O}\left(d^3 \log n\right)$ and $\mathcal{O}\left(d\, r^2 \log n\right)$ parameters resp.

Furthermore, we show that the assumption of semiseparability of order r can be relaxed to that of *quasi-separability of order* r. We establish the direct relation $r_k = s_k + 2$ between the $d-1$ *TT ranks* s_k of the matrix in question and the *matrix ranks* r_k of the $d-1$ leading off-diagonal submatrices of the diffusion tensor.

Keywords: low-rank representation, diffusion operator, Tensor Train (TT), virtual levels, Quantized Tensor Train (QTT), semiseparable matrices, quasi-separable matrices.
AMS Subject Classification: 15A69, 65F99.

1 Introduction

Recent surveys [1, 2] and the monograph [3] present a variety of *tensor decompositions*, i. e. low-parametric non-linear representations of high-dimensional arrays, which have been recently applied to the solution of PDEs with the aim to overcome the "curse of dimensionality" [4]. In the present paper, inspired primarily by financial market models, we consider d-dimensional matrices of the form

$$\begin{aligned}\mathbf{S}_d = \sum_{1\le k\le d} a_k^k\, Q_1 \otimes \ldots \otimes Q_{k-1} \otimes S_k \otimes Q_{k+1} \otimes \ldots \otimes Q_d \\ + \sum_{1\le p<q\le d} a_q^p\, Q_1 \otimes \ldots \otimes Q_{p-1} \otimes X_p \otimes Q_{p+1} \otimes \ldots \otimes Q_{q-1} \otimes Y_q \otimes Q_{q+1} \otimes \ldots \otimes Q_d \\ + \sum_{1\le p<q\le d} a_p^q\, Q_1 \otimes \ldots \otimes Q_{p-1} \otimes Y_p \otimes Q_{p+1} \otimes \ldots \otimes Q_{q-1} \otimes X_q \otimes Q_{q+1} \otimes \ldots \otimes Q_d.\end{aligned} \tag{1}$$

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Such a matrix arises, for example, from the discretization of a linear diffusion operator in divergence form

$$\mathcal{L} = -\sum_{p,q=1}^{d} \partial_q \, \kappa^{pq} \, \partial_p = -\nabla^\top \mathcal{K} \nabla, \tag{2}$$

in the unit cube $D = (0,1)^d$, $d \geq 3$, with homogeneous Dirichlet boundary conditions, where $\mathcal{K} = [\kappa^{pq}]_{p,q=1}^{d} : D \to \mathbb{R}^{d \times d}$ is a sufficiently smooth diffusion tensor.

Throughout this paper we assume that $\mathcal{K}$ is rank-1 separable (with respect to the spatial variables):

$$\kappa^{pq} = a_q^p \cdot \kappa_1^{pq} \otimes \ldots \otimes \kappa_d^{pq}, \quad 1 \leq p, q \leq d, \tag{3}$$

where the matrix $A = [a_q^p]_{p,q=1}^{d}$ is a symmetric scaling factor of the diffusion tensor, and that the coordinate factors are

$$\kappa_k^{pq} = \begin{cases} \widehat{\kappa}_k, & k = p = q, \\ \overline{\kappa}_k, & k = p \neq q \quad \text{or} \quad k = q \neq p, \\ \kappa_k, & \text{otherwise.} \end{cases} \tag{4}$$

We consider Galerkin finite element discretization (1) of $\mathcal{L}$ defined in (2). Due to the product structure of D, we use tensor-product shape functions $\psi_{i_1,\ldots,i_d} = \psi_{i_1}^1 \otimes \ldots \otimes \psi_{i_d}^d$, where $\psi_{i_k}^k$, $1 \leq i_k \leq n_k$ are the shape functions corresponding to the k-th coordinate, $1 \leq k \leq d$. Then the stiffness matrix with the entries

$$(\mathbf{S}_d)_{\substack{i_1,\ldots,i_d \\ j_1,\ldots,j_d}} = \langle \mathcal{L} \, \psi_{i_1,\ldots,i_d}, \, \psi_{j_1,\ldots,j_d} \rangle_{L_2(D)}, \quad 1 \leq i_k, j_k \leq n_k, \tag{5}$$

takes the form (1), where the coordinate factors are

$$\begin{aligned} (Q_k)_{\,i_k j_k} &= \int \kappa_k \cdot \quad \psi_{i_k}^{(k)} \cdot \quad \psi_{j_k}^{(k)}, & (S_k)_{\,i_k j_k} &= \int \widehat{\kappa}_k \cdot \nabla\psi_{i_k}^{(k)} \cdot \nabla\psi_{j_k}^{(k)}, \\ (X_k)_{\,i_k j_k} &= \int \overline{\kappa}_k \cdot \nabla\psi_{i_k}^{(k)} \cdot \quad \psi_{j_k}^{(k)}, & (Y_k)_{\,i_k j_k} &= \int \overline{\kappa}_k \cdot \quad \psi_{i_k}^{(k)} \cdot \nabla\psi_{j_k}^{(k)} \end{aligned}$$

for $1 \leq i_k, j_k \leq n_k$ and $1 \leq k \leq d$. Unlike the mass matrix, which arises in the rank-1 separable representation $\mathbf{M}_d = M_1 \otimes \ldots \otimes M_d$, where $(M_k)_{\,i_k j_k} = \int \psi_{i_k}^{(k)} \psi_{j_k}^{(k)}$, the stiffness matrix $\mathbf{S}_d$ given in (1), due to symmetry, comprises $\frac{1}{2}(d+1)d$ rank-1 terms.

In the present paper we construct explicit low-rank *Tensor Train* [5, 6] representations of $\mathbf{S}_d$. This means that we derive explicitly arrays U_k, $1 \leq k \leq d$, referred to as *TT cores*, such that the equality

$$\begin{aligned} (\mathbf{S}_d)_{\substack{i_1,\ldots,i_d \\ j_1,\ldots,j_d}} \quad = \quad & \sum_{\alpha_1=1}^{r_1} \ldots \sum_{\alpha_{d-1}=1}^{r_{d-1}} U_1(i_1, j_1, \alpha_1) \cdot U_2(\alpha_1, i_2, j_2, \alpha_2) \cdot \ldots \\ \cdot \quad & U_{d-1}(\alpha_{d-2}, i_{d-1}, j_{d-1}, \alpha_{d-1}) \cdot U_d(\alpha_{d-1}, i_d, j_d) \end{aligned} \tag{6}$$

holds elementwise and such that the summation limits $r_1, \ldots, r_{d-1}$, which are called *TT ranks* (or just *ranks*) of the decomposition (6), are moderate. We give a more detailed overview of the TT format in Section 2.

The main results of the present paper are the following. First, Corollary 3.3 presents a TT representation of $\mathbf{S}_d$ of ranks bounded by $2 + \left\lfloor \frac{d}{2} \right\rfloor$ and, thus, generalizes the corresponding result of [7, Lemma 5.1] from a diagonal diffusion tensor to that of the form (3)–(4). Second, Corollary 3.6 suggests a reduced decomposition of ranks bounded by $2 + r$, provided that A is *semiseparable of order* r (see, e. g., [8]). Third, Theorem 3.7 establishes the direct relation $r_k = s_k + 2$ between the $d-1$ *TT ranks* r_k of $\mathbf{S}_d$ and the *matrix ranks* s_k of the $d-1$ leading off-diagonal submatrices of A.

In Section 3 we obtain the results listed above for a general matrix of the form (1), see Lemma 3.2 and Lemma 3.5, and then specify them for the stiffness matrix obtained from a self-adjoint linear diffusion operator (2). In Section 4 we discuss how the results on the TT structure of $\mathbf{S}_d$ imply corresponding results on its *Quantized Tensor Train (QTT)* structure (a definition of the QTT representation is given in Section 2.4).

In Section 2.1 we discuss briefly the connection between the TT structure of a tensor and the low-rank structure of the *unfolding matrices* obtained from the tensor. Theorem 3.7, on the other hand, relates the TT structure of matrices of the form (1) to the *quasi-separable* (see, e. g., [9]) structure of A, which we regard a very interesting result.

Remark 1.1. *As practical examples involving diffusion tensors satisfying* (3)–(4) *we may consider high-dimensional option pricing problems under diffusion type market models. The case of a constant diffusion tensor $\mathcal{K} = A$ corresponds to the Black-Scholes market model after an appropriate change of variables. We may also consider more general market models of the diffusion type with $\kappa^{pq}(x_1, \ldots, x_d) = a^p_q \cdot \overline{\kappa}_p(x_p) \cdot \overline{\kappa}_q(x_q)$, where the functions $\overline{\kappa}_k$, $1 \le k \le d$, are sufficiently smooth. Financial models with such diffusion tensors are, e. g., the multi-dimensional Black-Scholes model in real price variables, see [10, 11], the Heston model or the multiscale stochastic volatility model, see [12]. In the case of the Black-Scholes model in real price in* (4) *we have $\widehat{\kappa}_k(x_k) = x_k^2$, $\overline{\kappa}_k(x_k) = x_k$ and $\kappa_k(x_k) = 1$ for $1 \le k \le d$, and for stochastic volatility models these coordinate factors have a more involved form.*

Remark 1.2. *Consider bead-spring chain models with FENE-type potentials, which arise from the kinetic theory of dilute polymer solutions (see [13] and references therein). Such models lead to high-dimensional Fokker-Planck equations with diffusion terms of the form* (2)–(4)*. For example, see [13, (1.9)]: there a diffusion operator with respect to the conformation vectors of springs (which model the polymer in question) is considered. It can be decomposed into a diffusion operator of the form* (2)–(4)*, which we analyze in the present paper, and a drift term, the low-rank TT structure of which follows from [7, Lemma 5.1]. In view of this, let us emphasize that the results of the present paper, related to the TT structure of discretizations of diffusion operators, apply straightforwardly to the cases when the domain D has a more complicated structure: the coordinates of D need not be Cartesian coordinates, and D may be a Cartesian product of spheres, tori or other manifolds.*

2 The TT and QTT representations, notation

2.1 The TT decomposition

The *Tensor Train (TT)* decomposition of high-dimensional tensors was proposed by Oseledets and Tyrtyshnikov, see [5, 6]. Let us recall that a d-dimensional $n_1 \times \ldots \times n_d$-vector $\mathbf{z}$ is said to be represented in the TT format with *TT ranks* $r_1, \ldots, r_{d-1}$ in terms of *TT cores* $U_1 \in \mathbb{R}^{n_1 \times r_1}, U_2 \in \mathbb{R}^{r_1 \times n_2 \times r_2}, \ldots, U_{d-1} \in \mathbb{R}^{r_{d-2} \times n_{d-1} \times r_{d-1}}, U_d \in \mathbb{R}^{r_{d-1} \times n_d}$, if

$$\mathbf{z}_{i_1,\ldots,i_d} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} U_1(i_1, \alpha_1) \cdot U_2(\alpha_1, i_2, \alpha_2) \cdot \ldots \cdot U_{d-1}(\alpha_{d-2}, i_{d-1}, \alpha_{d-1}) \cdot U_d(\alpha_{d-1}, i_d) \tag{7}$$

holds for $1 \le i_k \le n_k$, where $1 \le k \le d$. The TT cores are arrays with one of d *mode indices* i_k and two subsequent or only one of $d-1$ rank indices α_k. For every $k = 1, \ldots, d-1$ Equation (7) implies a rank-r_k representation of the corresponding unfolding matrix $Z^{(k)}$ with entries defined as follows:

$$Z^{(k)}{}_{i_1 \ldots i_k;\, i_{k+1} \ldots i_d} = \mathbf{z}_{i_1 \ldots i_d}. \tag{8}$$

Conversely, exact or approximate low-rank structure of the unfolding matrices yields the same TT structure of the vector, see [6, Theorem 2.1 and Theorem 2.3]. This relation of the TT ranks to the matrix ranks of certain matrices allows for robust TT-structured computations based on standard matrix algorithms, such as SVD and QR, see [6] for details.

The TT decomposition can be applied similarly to a d-dimensional matrix (a block matrix with d levels) of size $(m_1 \times \ldots \times m_d) \times (n_1 \times \ldots \times n_d)$; for instance, see (6). In this case every mode index i_k is accompanied by another mode index j_k; and Tensor Train cores and ranks, as well as unfolding matrices, are defined analogously. This particular way of representing matrices in the TT format (instead of, say, applying the decomposition to a $2d$-dimensional vectorization of a matrix) is motivated by the desired efficiency of computations with TT-structured matrices; for further details refer to the discussion of the matrix-vector multiplication in [6, Section 4.3].

2.2 Core matrices and the strong Kronecker product

Following [7], we use the following notation for TT cores and operations with them.

Consider a core U_k of rank $r_{k-1} \times r_k$ and mode size $m_k \times n_k$ from a TT representation (for example, (6)) of a matrix. Assume that $m_k \times n_k$-matrices $G_{\alpha\beta}$, $\alpha = 1, \ldots, r_{k-1}$, $\beta = 1, \ldots, r_k$ are *TT blocks* of the core U_k, i. e. $U_k(\alpha, i_k, j_k, \beta) = (G_{\alpha\beta})_{i_k j_k}$ for all values of rank indices α, β and mode indices i_k, j_k. We consider the core U_k as an $r_{k-1} \times r_k$-matrix, which we refer to as the *core matrix* of U_k:

$$U_k = \begin{bmatrix} G_{11} & \cdots & G_{1r_k} \\ \vdots & \vdots & \vdots \\ G_{r_{k-1}1} & \cdots & G_{r_{k-1}r_k} \end{bmatrix}. \tag{9}$$

In order to avoid confusion we use parentheses for ordinary matrices, whose entries are numbers, multiplied as usual, and square brackets for cores (core matrices), whose entries are blocks, multiplied by means of the strong Kronecker product "$\bowtie$" defined below. Addition of cores is meant elementwise. Also, we may think of $G_{\alpha\beta}$ or of any submatrix of the core matrix in (9) as *subcores* of U_k.

Throughout the present paper we omit the indices in TT decompositions like (6) with the help of the *strong Kronecker product* [14]. In order to avoid the confusion with the Hadamard and tensor products, we denote this operation by "$\bowtie$", as in [7, Definition 2.1], where it was introduced as follows specifically for connecting cores into "tensor trains".

Definition 2.1 (Strong Kronecker product of TT cores). *Consider cores U_1 and U_2 of ranks $r_0 \times r_1$ and $r_1 \times r_2$ and of mode sizes $m_1 \times n_1$ and $m_2 \times n_2$ respectively, composed of blocks $G^{(1)}_{\alpha_0\alpha_1}$ and $G^{(2)}_{\alpha_1\alpha_2}$, $1 \le \alpha_k \le r_k$ for $0 \le k \le 2$. Let us define the* strong Kronecker product *$U_1 \bowtie U_2$ of U_1 and U_2 as a core of rank $r_0 \times r_2$ and mode size $m_1 m_2 \times n_1 n_2$, consisting of blocks*

$$G_{\alpha_0\alpha_2} = \sum_{\alpha_1=1}^{r_1} G^{(1)}_{\alpha_0\alpha_1} \otimes G^{(2)}_{\alpha_1\alpha_2}, \quad 1 \le \alpha_0 \le r_0, \quad 1 \le \alpha_2 \le r_2.$$

In other words, we define $U_1 \bowtie U_2$ as a usual matrix product of the corresponding core matrices, their entries (blocks) being multiplied by means of the Kronecker (tensor) product. For example,

$$\begin{bmatrix} G_{11} & G_{12} \\ G_{21} & G_{22} \end{bmatrix} \bowtie \begin{bmatrix} H_{11} & H_{12} \\ H_{21} & H_{22} \end{bmatrix} = \begin{bmatrix} G_{11} \otimes H_{11} + G_{12} \otimes H_{21} & G_{11} \otimes B_{12} + G_{12} \otimes H_{22} \\ G_{21} \otimes H_{11} + G_{22} \otimes H_{21} & G_{21} \otimes B_{12} + G_{22} \otimes H_{22} \end{bmatrix}.$$

Then equation (7) can be revised as

$$\mathbf{S}_d = U_1 \bowtie U_2 \bowtie \ldots \bowtie U_{d-1} \bowtie U_d. \tag{10}$$

If we consider two matrices $\mathbf{P} = V_1 \bowtie \ldots \bowtie V_d$ and $\mathbf{Q} = W_1 \bowtie \ldots \bowtie W_d$, their tensor product can be written as $\mathbf{P} \otimes \mathbf{Q} = V_1 \bowtie \ldots \bowtie V_d \bowtie W_1 \bowtie \ldots \bowtie W_d$. Once the matrices have the same mode size, a linear combination of them reads

$$\alpha \mathbf{P} + \beta \mathbf{Q} = \begin{bmatrix} V_1 & W_1 \end{bmatrix} \bowtie \operatorname{diag}\left[V_2, W_2\right] \bowtie \ldots \bowtie \operatorname{diag}\left[V_{d-1}, W_{d-1}\right] \bowtie \begin{bmatrix} \alpha V_d \\ \beta W_d \end{bmatrix},$$

where we use $\operatorname{diag}\left[U_1, \ldots, U_t\right]$ to denote a block-diagonal core composed of the cores $U_1, \ldots, U_t$ as subcores, so that

$$\operatorname{diag}\left[V_k, W_k\right] = \begin{bmatrix} V_k & \\ & W_k \end{bmatrix}.$$

Throughout the paper we leave zero blocks blank, as in the last equation.

2.3 Explicit rank reduction

In Section 2.1 we mentioned the relation between the TT ranks of a vector (matrix) and the unfolding matrices of the vector (matrix). Due to this relation, reducing a TT decomposition (i. e. its ranks) means removing a linear dependence from low-rank representations of the unfolding matrices, implied by (7), (6). This can be done by the standard transformations of rows and columns in the core matrices: the strong Kronecker product inherits the basic properties of the matrix and Kronecker (tensor) products; for instance,

$$\begin{aligned} &\begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \bowtie \begin{bmatrix} \alpha W_{11} & \alpha W_{12} \\ \beta W_{11} & \beta W_{12} \end{bmatrix} = \begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \bowtie \left(\begin{bmatrix} \alpha \\ \beta \end{bmatrix} \bowtie \begin{bmatrix} W_{11} & W_{12} \end{bmatrix} \right) \\ &= \left(\begin{bmatrix} V_{11} & V_{12} \\ V_{21} & V_{22} \end{bmatrix} \bowtie \begin{bmatrix} \alpha \\ \beta \end{bmatrix} \right) \bowtie \begin{bmatrix} W_{11} & W_{12} \end{bmatrix} = \begin{bmatrix} \alpha V_{11} + \beta V_{12} \\ \alpha V_{21} + \beta V_{22} \end{bmatrix} \bowtie \begin{bmatrix} W_{11} & W_{12} \end{bmatrix} \end{aligned} \tag{11}$$

for any coefficients α, β and blocks *or* subcores $V_{11}, V_{12}, V_{21}, V_{22}, W_{11}, W_{12}$ of compatible ranks and mode sizes. Equality (11) illustrates the basic decomposition technique which we use routinely throughout the paper.

2.4 The QTT decomposition

With the aim of further reduction of the complexity, the TT format can be applied to a "quantized" vector (matrix), which leads to the *Quantized Tensor Train* (QTT) format [15, 16, 17]. The idea of quantization of the k-th "physical" dimension consists in replacing it with l_k "virtual" dimensions (levels) [18], provided that the corresponding mode size n_k can be factorized as $n_k = n_{k1} \cdot n_{k2} \cdot \ldots \cdot n_{kl_k}$ in terms of integral factors $n_{km_k} \geq 2$, $m_k = 1, \ldots, l_k$. This corresponds to reshaping the k-th mode of size n_k into l_k modes of sizes $n_{k1}, \ldots, n_{kl_k}$.

Compared to the TT decomposition (without quantization), the QTT format represents more structure in the data by splitting all the "virtual" dimensions introduced. It involves additional rank numbers, and they can be higher. Typically, one tends to introduce as fine (i. e. with small n_{km_k}) quantization as possible and wind up with as many virtual modes as possible. This corresponds to seeking as much low-rank QTT structure in the data as possible.

As an example of the finest possible quantization one may consider the representation of every "physical" scalar index $i = \overline{i_1, \ldots, i_l} \equiv 1 + \sum_{k=1}^{l} 2^{l-k} (i_k - 1)$ varying from 1 to 2^l in terms of "virtual" indices $i_1, \ldots, i_l$ taking values 1 and 2. This binary encoding reshapes a one-dimensional 2^l-component vector into an l-dimensional $2 \times \ldots \times 2$-tensor; and a d-dimensional $2^{l_1} \times \ldots \times 2^{l_d}$-tensor into an $l_1 + \ldots + l_d$-dimensional $2 \times \ldots \times 2$-tensor.

A TT decomposition of a vector (matrix) under such a transformation is referred to as a *QTT decomposition* of the vector (matrix). The TT ranks of this decomposition are called *QTT ranks*. In this sense (7) and (6), with d being replaced with l, also present QTT decompositions of ranks $r_1, \ldots, r_{l-1}$ of a one-dimensional vector $\hat{\mathbf{z}}$ and of a one-dimensional matrix $\hat{\mathbf{S}}_d$ with entries $\hat{\mathbf{z}}_{\overline{i_1,\ldots,i_l}} = \mathbf{z}_{i_1,\ldots,i_l}$ and $\left(\hat{\mathbf{S}}_d\right)_{\overline{i_1,\ldots,i_l},\overline{j_1,\ldots,j_l}} = (\mathbf{S}_d)_{i_1,\ldots,i_l,j_1,\ldots,j_l}$.

The computational efficiency of the TT, QTT and Hierarchical Tensor [19, 20] representations has been demonstrated in many papers, including [21, 22, 23] on elliptic PDEs and eigenvalue problems, [24, 25, 26] on parabolic PDEs, [27] on nonlinear EVPs, [28] on multi-parametric problems, [29] on stochastic PDEs, [30] on problems in quantum molecular dynamics.

3 Low-rank TT structure of the diffusion operator

3.1 Diagonal diffusion tensor

Assume first that $a_q^p = 0$ for $p \neq q$ in (1). Then the stiffness matrix takes the form

$$\mathbf{S}_d = \sum_{k=1}^{d} Q_1 \otimes \ldots \otimes Q_{k-1} \otimes S_k \otimes Q_{k+1} \otimes \ldots \otimes Q_d. \tag{12}$$

Consider also the matrix $\mathbf{Q}_d = Q_1 \otimes \ldots \otimes Q_d$, which coincides with the mass matrix in case $\kappa_k = 1$ in (4). The common TT structure of $\mathbf{Q}_d$ and $\mathbf{S}_d$ was studied in [7, Lemma 5.1] and can be described as follows.

Proposition 3.1. *Let $d \geq 2$. Then the following TT representation of ranks $2, \ldots, 2$ in terms of Q_k and S_k, $1 \leq k \leq d$, holds true:*

$$\begin{bmatrix} \mathbf{Q}_d \\ \mathbf{S}_d \end{bmatrix} = W_1 \bowtie W_2 \bowtie \ldots \bowtie W_{d-1} \bowtie V_d,$$

where the cores are

$$W_k = \begin{bmatrix} Q_k & \\ S_k & Q_k \end{bmatrix} \quad \textit{and} \quad V_d = \begin{bmatrix} Q_d \\ S_d \end{bmatrix}.$$

In order to represent $\mathbf{S}_d$ only, one leaves out the first row in W_1.

3.2 Non-diagonal diffusion tensor

In this section we generalize Proposition 3.1 to the form (1) of the matrix $\mathbf{S}_d$ with a non-diagonal diffusion tensor: we show that the core $\begin{bmatrix} \mathbf{Q}_d \\ \mathbf{S}_d \end{bmatrix}$ can be represented in the TT format in terms of the matrices Q_k, S_k, X_k, Y_k, $1 \leq k \leq d$, and coefficients a_q^p, $1 \leq p, q \leq d$, with ranks increasing linearly from 4 to $2 + 2\left\lfloor \frac{d}{2} \right\rfloor$ and then decreasing linearly from $2 + 2(d - \left\lfloor \frac{d}{2} \right\rfloor - 1)$ to 4 from left to right, i. e. bounded by $\left\lfloor \frac{d}{2} \right\rfloor$.

For the presentation of our calculations and results, let us introduce the following cores: for $2 \leq k \leq d-1$

$$F_k = \begin{bmatrix} a_{k+1}^k X_k & \cdots & a_d^k X_k \end{bmatrix} \quad \text{and} \quad G_k = \begin{bmatrix} a_k^{k+1} Y_k & \cdots & a_k^d Y_k \end{bmatrix}$$

are cores of rank $1 \times d-k$; $\Sigma_k = \operatorname{diag}[Q_k, \ldots, Q_k]$ and $\Omega_k = \operatorname{diag}[Q_k, \ldots, Q_k]$ are diagonal cores of rank $k-1 \times k-1$ and $d-k \times d-k$ respectively;

$$P_k = \begin{bmatrix} a_k^1 Y_k \\ \vdots \\ a_k^{k-1} Y_k \end{bmatrix} \quad \text{and} \quad R_k = \begin{bmatrix} a_1^k X_k \\ \vdots \\ a_{k-1}^k X_k \end{bmatrix}$$

are cores of rank $k-1 \times 1$;

$$M_k = \begin{bmatrix} a_{k+1}^1 Q_k & \cdots & a_d^1 Q_k \\ \vdots & \vdots & \vdots \\ a_{k+1}^{k-1} Q_k & \cdots & a_d^{k-1} Q_k \end{bmatrix} \quad \text{and} \quad N_k = \begin{bmatrix} a_1^{k+1} Q_k & \cdots & a_1^d Q_k \\ \vdots & \vdots & \vdots \\ a_{k-1}^{k+1} Q_k & \cdots & a_{k-1}^d Q_k \end{bmatrix}$$

are cores of rank $k-1 \times d-k$.

Lemma 3.2. *For any $d \geq 3$ and r such that $1 \leq r \leq d-2$ the following TT representation holds true:*

$$\begin{bmatrix} \mathbf{Q}_d \\ \mathbf{S}_d \end{bmatrix} = U_1 \bowtie U_2 \bowtie \ldots \bowtie U_r \bowtie W_{r+1} \bowtie V_{r+2} \bowtie \ldots \bowtie V_{d-1} \bowtie V_d, \tag{13}$$

where the TT ranks are $4, 6, \ldots, 2+2r,\ 2+2(d-r-1), \ldots, 6, 4$. The cores involved are the following:

$$U_1 = \begin{bmatrix} Q_1 & & & \\ a_1^1 S_1 & Q_1 & X_1 & Y_1 \end{bmatrix}, \quad V_d = \begin{bmatrix} Q_d \\ a_d^d S_d \\ Y_d \\ X_d \end{bmatrix}, \quad V_k = \begin{bmatrix} Q_k & & & \\ a_k^k S_k & Q_k & F_k & G_k \\ Y_k & & & \\ & & \Omega_k & \\ X_k & & & \\ & & & \Omega_k \end{bmatrix},$$

$$W_k = \begin{bmatrix} Q_k & & & \\ a_k^k S_k & Q_k & F_k & G_k \\ P_k & & M_k & \\ R_k & & & N_k \end{bmatrix}, \quad U_k = \begin{bmatrix} Q_k & & & \\ a_k^k S_k & Q_k & X_k & Y_k \\ P_k & & \Sigma_k & \\ R_k & & & \Sigma_k \end{bmatrix} \tag{14}$$

for $2 \leq k \leq d-1$. Here U_k is of rank $2+2(k-1) \times 2+2k$; W_k, of rank $2+2(k-1) \times 2+2(d-k)$; V_k, of rank $4+2(d-k) \times 2+2(d-k)$.

Proof. In order to make the proof clearer and less technical, we give it for the case of an upper triangular matrix A, when the third sum in (1) cancels out, the cores G_k, R_k and N_k become trivial and the cores of the decomposition (13) reduce to

$$U_1 = \begin{bmatrix} Q_1 & & \\ a_1^1 S_1 & Q_1 & X_1 \end{bmatrix}, \quad V_d = \begin{bmatrix} Q_d \\ a_d^d S_d \\ Y_d \end{bmatrix}, \quad V_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & F_k \\ Y_k & & \\ & & \Omega_k \end{bmatrix},$$

$$W_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & F_k \\ P_k & & M_k \end{bmatrix}, \quad U_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & X_k \\ P_k & \Sigma_k & \end{bmatrix} \tag{15}$$

for $2 \leq k \leq d-1$. Here U_k is of rank $2+k-1 \times 2+k$; W_k, of rank $2+k-1 \times 2+d-k$; V_k, of rank $4+d-k \times 2+d-k$.

In the general case the proof can be obtained directly in the very same way.

Backward sweep from d to 1. Let us consider the matrices $\boldsymbol{\mathcal{Q}}_k = Q_1 \otimes \ldots \otimes Q_k$ and

$$\boldsymbol{\mathcal{S}}_k = \sum_{1 \leq p \leq k} a_p^p \, Q_1 \otimes \ldots \otimes Q_{p-1} \otimes S_p \otimes Q_{p+1} \otimes \ldots \otimes Q_p$$
$$+ \sum_{1 \leq p < q \leq k} a_q^p \, Q_1 \otimes \ldots \otimes Q_{p-1} \otimes X_p \otimes Q_{p+1} \otimes \ldots \otimes Q_{q-1} \otimes Y_q \otimes Q_{q+1} \otimes \ldots \otimes Q_k$$

for $1 \leq k \leq d$. Then for $2 \leq k \leq d$ we have the recursive relations

$$\boldsymbol{\mathcal{Q}}_k \quad = \quad \boldsymbol{\mathcal{Q}}_{k-1} \otimes Q_k,$$

$$\boldsymbol{\mathcal{S}}_k \quad = \quad \boldsymbol{\mathcal{S}}_{k-1} \otimes Q_k + \boldsymbol{\mathcal{Q}}_{k-1} \otimes a_k^k\, S_k + \boldsymbol{\mathcal{X}}_{k-1}^k \otimes Y_k, \tag{16}$$

where

$$\boldsymbol{\mathcal{X}}_k^q \quad = \quad \sum_{p=1}^{k} Q_1 \otimes \ldots \otimes Q_{p-1} \otimes a_q^p\, X_p \otimes Q_{p+1} \otimes \ldots \otimes Q_k \tag{17}$$

for $1 \le k < q \le d$. Let us now define the core

$$\tilde{U}_k = \begin{bmatrix} \boldsymbol{\mathcal{Q}}_k & & & & \\ \boldsymbol{\mathcal{S}}_k & \boldsymbol{\mathcal{Q}}_k & \boldsymbol{\mathcal{X}}_k^{k+1} & \cdots & \boldsymbol{\mathcal{X}}_k^d \end{bmatrix}$$

of rank $2 \times 2 + (d-k)$ for $1 \le k \le d-1$. Then, in particular, (16) for $k = d$ can be recast with the use of the strong Kronecker product as

$$\begin{bmatrix} \mathbf{Q}_d \\ \mathbf{S}_d \end{bmatrix} = \tilde{U}_{d-1} \bowtie V_d. \tag{18}$$

The matrices defined by (17) for $2 \le k < q \le d$ satisfy $\boldsymbol{\mathcal{X}}_k^q = \boldsymbol{\mathcal{X}}_{k-1}^q \otimes Q_k + \boldsymbol{\mathcal{Q}}_{k-1} \otimes a_q^k\, X_k$, from which we obtain for $2 \le k \le d$ that

$$\begin{bmatrix} \boldsymbol{\mathcal{X}}_k^{k+1} & \cdots & \boldsymbol{\mathcal{X}}_k^d \end{bmatrix} = \begin{bmatrix} \boldsymbol{\mathcal{Q}}_{k-1} & \boldsymbol{\mathcal{X}}_{k-1}^{k+1} & \cdots & \boldsymbol{\mathcal{X}}_{k-1}^d \end{bmatrix} \bowtie \begin{bmatrix} F_k \\ \Omega_k \end{bmatrix}. \tag{19}$$

Equations (16) and (19) result in the recursive TT structure of $\tilde{U}_k$:

$$\begin{aligned} \tilde{U}_k \quad &= \quad \begin{bmatrix} \boldsymbol{\mathcal{Q}}_{k-1} & & & & & & & & \\ & \boldsymbol{\mathcal{S}}_{k-1} & \boldsymbol{\mathcal{Q}}_{k-1} & \boldsymbol{\mathcal{X}}_{k-1}^k & \boldsymbol{\mathcal{Q}}_{k-1} & \boldsymbol{\mathcal{Q}}_{k-1} & \boldsymbol{\mathcal{X}}_{k-1}^{k+1} & \cdots & \boldsymbol{\mathcal{X}}_{k-1}^d \end{bmatrix} \\ &\bowtie \begin{bmatrix} Q_k & & \\ Q_k & & \\ a_k^k S_k & & \\ Y_k & & \\ & Q_k & \\ & & F_k \\ & & \Omega_k \end{bmatrix} \\ &= \begin{bmatrix} \boldsymbol{\mathcal{Q}}_{k-1} & & & & & \\ \boldsymbol{\mathcal{S}}_{k-1} & \boldsymbol{\mathcal{Q}}_{k-1} & \boldsymbol{\mathcal{X}}_{k-1}^k & \boldsymbol{\mathcal{X}}_{k-1}^{k+1} & \cdots & \boldsymbol{\mathcal{X}}_{k-1}^d \end{bmatrix} \bowtie \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & F_k \\ Y_k & & \\ & & \Omega_k \end{bmatrix}, \end{aligned}$$

i. e. $\tilde{U}_k = \tilde{U}_{k-1} \bowtie V_k$ for $2 \le k \le d-1$. By expanding this recursion leftwards, we obtain the TT representation

$$\begin{bmatrix} \mathbf{Q}_d \\ \mathbf{S}_d \end{bmatrix} = \tilde{U}_1 \bowtie V_2 \bowtie \ldots \bowtie V_{d-1} \bowtie V_d \tag{20}$$

of ranks $d+1, d, \ldots, 4, 3$.

Direct sweep from 1 **to** r**.** The first factor of the decomposition (20) contains many linearly dependent columns. Indeed, as long as $\boldsymbol{\mathcal{X}}_1^q = a_q^1 X_1$ for $1 < q \le d$, we have

$$\tilde{U}_1 = U_1 \bowtie T_1 \quad \text{with} \quad T_1 = \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & a_2^1 & \cdots & a_d^1 \end{bmatrix}, \tag{21}$$

where T_1 is a core of rank $2 + 1 \times 2 + d - 1$. Now for $1 \le k \le r+1$ we compose the cores

$$\Theta_k = \begin{bmatrix} a_{k+1}^1 & \cdots & a_d^1 \\ \vdots & \vdots & \vdots \\ a_{k+1}^k & \cdots & a_d^k \end{bmatrix} \quad \text{and} \quad T_k = \begin{bmatrix} 1 & & \\ & 1 & \\ & & \Theta_k \end{bmatrix}$$

of rank $k \times d-k$ and $2+k \times 2+d-k$ respectively. Note that for $2 \le k \le r+1$

$$\Theta_{k-1} \bowtie \begin{bmatrix} Y_k \\ \\ \\ \end{bmatrix} = P_k, \quad \Theta_{k-1} \bowtie \begin{bmatrix} \\ \Omega_k \end{bmatrix} = M_k,$$

which allows us to conclude that

$$T_{k-1} \bowtie V_k = \begin{bmatrix} 1 & & \\ & 1 & \\ & & \Theta_{k-1} \end{bmatrix} \bowtie \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & F_k \\ Y_k & & \\ & & \Omega_k \\ X_k & & \end{bmatrix} = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & F_k \\ P_k & & M_k \end{bmatrix} = W_k \tag{22}$$

for $2 \le k \le r+1$. Also, for the same range of k we may see that

$$\begin{aligned} \begin{bmatrix} F_k \\ M_k \end{bmatrix} &= \begin{bmatrix} a_{k+1}^k X_k & \cdots & a_d^k X_k \\ a_{k+1}^1 Q_k & \cdots & a_d^1 Q_k \\ \vdots & \vdots & \vdots \\ a_{k+1}^{k-1} Q_k & \cdots & a_d^{k-1} Q_k \end{bmatrix} = \begin{bmatrix} & & X_k \\ Q_k & & \\ & \ddots & \\ & & Q_k \end{bmatrix} \bowtie \Theta_k \\ &= \begin{bmatrix} & X_k \\ \Sigma_k & \end{bmatrix} \bowtie \Theta_k, \end{aligned} \tag{23}$$

so that we may extract T_k as a factor on the right:

$$W_k = \begin{bmatrix} Q_k & & & \\ a_k^k S_k & Q_k & & X_k \\ P_k & & \Sigma_k & \end{bmatrix} \bowtie \begin{bmatrix} 1 & & \\ & 1 & \\ & & \Theta_k \end{bmatrix} = U_k \bowtie T_k, \tag{24}$$

which holds for $2 \le k \le d-1$. Ultimately, by applying (21) and the successive transformations (22), (24) for $2 \le k \le r+1$ to (20), we obtain the decomposition

$$\begin{bmatrix} \mathbf{Q}_d \\ \mathbf{S}_d \end{bmatrix} = U_1 \bowtie U_2 \bowtie \ldots \bowtie U_r \bowtie W_{r+1} \bowtie V_{r+2} \bowtie \ldots \bowtie V_{d-1} \bowtie V_d.$$

□

Let us now consider the particular case when A is symmetric and $Y_k = \omega X_k$ for $1 \le k \le d$ with some $\omega \in \mathbb{R}$. This holds true with $\omega = -1$ if the coordinate factors $\overline{\kappa}_k$ in (4) are constant.

Corollary 3.3. *Assume that $d \ge 3$, A is symmetric and, for some $\omega \in \mathbb{R}$, $Y_k = \omega X_k$ for $1 \le k \le d$ in* (1)*. Then for any r such that $1 \le r \le d-2$ the following TT representation holds true:*

$$\begin{bmatrix} \mathbf{Q}_d \\ \mathbf{S}_d \end{bmatrix} = U_1 \bowtie U_2 \bowtie \ldots \bowtie U_r \bowtie W_{r+1} \bowtie V_{r+2} \bowtie \ldots \bowtie V_{d-1} \bowtie V_d, \tag{25}$$

where the TT ranks are $3, 4, \ldots, 2+r,\ 2+(d-r-1), \ldots, 4, 3$. The cores involved are the following:

$$U_1 = \begin{bmatrix} Q_1 & & \\ a_1^1 S_1 & Q_1 & X_1 \end{bmatrix}, \quad V_d = \begin{bmatrix} Q_d \\ a_d^d S_d \\ X_d \end{bmatrix}, \quad V_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & 2\omega F_k \\ X_k & & \\ & & \Omega_k \end{bmatrix},$$

$$W_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & 2\omega F_k \\ 2\omega R_k & & 2\omega M_k \end{bmatrix}, \quad U_k = \begin{bmatrix} Q_k & & & \\ a_k^k S_k & Q_k & & X_k \\ 2\omega R_k & & \Sigma_k & \end{bmatrix} \tag{26}$$

for $2 \le k \le d-1$. Here U_k is of rank $2+k-1 \times 2+k$; W_k, of rank $2+k-1 \times 2+d-k$; V_k, of rank $4+d-k \times 2+d-k$.

Proof. From (1) we see that, under the assumptions of the corollary, $\mathbf{S}_d$ does not change if we replace Y_k with X_k and a_q^p, with $2\omega a_q^p$ for $p < q$ and 0 for $p > q$. By doing so we reduce the statement to the case of an upper triangular matrix A, considered in detail in Lemma 3.2. □

The representation suggested by Lemma 3.2 has the lowest ranks when $r = \left\lfloor \frac{d}{2} \right\rfloor$: if $d = 2r + 1$, where $r \geq 1$, then it is of ranks $4, 6, \ldots, 2r + 2, 2r + 2, \ldots, 6, 4$; if $d = 2r$, where $r \geq 2$, then its ranks are $4, 6, \ldots, 2r + 2, 2r, \ldots, 6, 4$. In both the cases the TT ranks of the decomposition proven are bounded by $2 + 2\left\lfloor \frac{d}{2} \right\rfloor$. A similar remark resulting in the upper bound $2 + \left\lfloor \frac{d}{2} \right\rfloor$ applies to Corollary 3.3.

3.3 Non-diagonal diffusion tensor with low-rank structure

When the scaling factor A of the diffusion tensor has a certain low-rank structure, the results of Lemma 3.2 and Corollary 3.3 may be remarkably refined. To start with, we assume the following.

Assumption 3.4. *The strictly upper and lower triangular parts of the matrix A involved in* (1) *have the following rank-r representations for some $r \leq \left\lfloor \frac{d}{2} \right\rfloor$:*

$$a_q^p = \sum_{\alpha=1}^{r} \xi_\alpha^p \eta_q^\alpha \quad \textit{for} \quad p < q \quad \textit{and} \quad a_q^p = \sum_{\alpha=1}^{r} \chi_\alpha^p \zeta_q^\alpha \quad \textit{for} \quad p > q$$

with $\xi_\alpha^p, \eta_q^\alpha, \chi_\alpha^p, \zeta_q^\alpha \in \mathbb{R}$, i. e. A is semiseparable of order r *(see, e. g., [8])*

Below we show that under this assumption we may modify the TT decomposition (13) and cut the TT ranks at $2 + 2r$, so that they still increase linearly from 4 to $2 + 2r$ from both the ends towards the middle of the decomposition, but then remain equal to $2 + 2r$ in the middle part. The same applies to Corollary 3.3, which results in a TT decomposition of ranks bounded by $2 + r$.

Let us introduce the cores

$$\overleftarrow{M}_{r+1} = \begin{bmatrix} \xi_1^1 Q_{r+1} & \cdots & \xi_r^1 Q_{r+1} \\ \vdots & \vdots & \vdots \\ \xi_1^r Q_{r+1} & \cdots & \xi_r^r Q_{r+1} \end{bmatrix}, \quad \overleftarrow{N}_{r+1} = \begin{bmatrix} \chi_1^1 Q_{r+1} & \cdots & \chi_1^r Q_{r+1} \\ \vdots & \vdots & \vdots \\ \chi_r^1 Q_{r+1} & \cdots & \chi_r^r Q_{r+1} \end{bmatrix}$$

of rank $r \times r$ and, for $r + 1 \leq k \leq d - r$, the following cores:

$$\Lambda_k = \begin{bmatrix} Q_k & & \\ & \ddots & \\ & & Q_k \end{bmatrix}, \quad \overline{P}_k = \begin{bmatrix} \eta_k^1 Y_k \\ \vdots \\ \eta_k^r Y_k \end{bmatrix} \quad \text{and} \quad \overline{R}_k = \begin{bmatrix} \zeta_1^k X_k \\ \vdots \\ \zeta_r^k X_k \end{bmatrix}$$

of rank $r \times r$, $r \times 1$ and $r \times 1$ respectively;

$$\overline{F}_k = \begin{bmatrix} \xi_1^k X_k & \cdots & \xi_r^k X_k \end{bmatrix} \quad \text{and} \quad \overline{G}_k = \begin{bmatrix} \chi_k^1 Y_k & \cdots & \chi_k^r Y_k \end{bmatrix}$$

of rank $1 \times r$;

$$\overrightarrow{M}_k = \begin{bmatrix} \eta_{k+1}^1 Q_k & \cdots & \eta_d^1 Q_k \\ \vdots & \vdots & \vdots \\ \eta_{k+1}^r Q_k & \cdots & \eta_d^r Q_k \end{bmatrix}, \quad \overrightarrow{N}_k = \begin{bmatrix} \zeta_1^{k+1} Q_k & \cdots & \zeta_1^d Q_k \\ \vdots & \vdots & \vdots \\ \zeta_r^{k+1} Q_k & \cdots & \zeta_r^d Q_k \end{bmatrix}$$

of rank $r \times d - k$.

Lemma 3.5. *Let $d \geq 5$ and Assumption 3.4 be valid. Then the following TT representation holds true:*

$$\begin{aligned}\begin{bmatrix}\mathbf{Q}_d \\ \mathbf{S}_d\end{bmatrix} &= U_1 \bowtie U_2 \bowtie \ldots \bowtie U_r \bowtie \overleftarrow{W}_{r+1} \bowtie \overline{W}_{r+2} \\ &\quad \bowtie \ldots \bowtie \overline{W}_{d-r-1} \bowtie \overrightarrow{W}_{d-r} \bowtie V_{d-r+1} \bowtie \ldots \bowtie V_{d-1} \bowtie V_d,\end{aligned} \tag{27}$$

where the TT ranks are $4, 6, \ldots, 2+2r,\ \ldots 2+2r \ldots,\ 2+2r, \ldots, 6, 4$. The cores involved are the following: U_k and V_k are the same as in (14)*,*

$$\overleftarrow{W}_{r+1} = \begin{bmatrix} Q_{r+1} & & & \\ a_{r+1}^{r+1} S_{r+1} & Q_{r+1} & \overline{F}_{r+1} & \overline{G}_{r+1} \\ P_{r+1} & & \overleftarrow{M}_{r+1} & \\ R_{r+1} & & & \overleftarrow{N}_{r+1} \end{bmatrix} \tag{28}$$

is a core of rank $2+2r \times 2+2r$ and, for $r+2 \leq k \leq d-r$,

$$\overline{W}_k = \begin{bmatrix} Q_k & & & \\ a_k^k S_k & Q_k & \overline{F}_k & \overline{G}_k \\ \overline{P}_k & & \Lambda_k & \\ \overline{R}_k & & & \Lambda_k \end{bmatrix} \quad \text{and} \quad \overrightarrow{W}_k = \begin{bmatrix} Q_k & & & \\ a_k^k S_k & Q_k & F_k & G_k \\ \overline{P}_k & & \overrightarrow{M}_k & \\ \overline{R}_k & & & \overrightarrow{N}_k \end{bmatrix} \tag{29}$$

are cores of rank $2+2r \times 2+2r$ and $2+2r \times 2+2(d-k)$ respectively.

Proof. As we do with Lemma 3.2, we give the proof for the case of an upper triangular matrix A. Then the third sum in (1) cancels out; the cores $\overleftarrow{N}_{r+1}$ and all $\overline{G}_k$, $\overline{R}_k$ and $\overrightarrow{N}_k$, as well as G_k, R_k and N_k, become trivial. As a consequence, the decomposition (27) involves U_k and V_k from (15) and the following cores:

$$\overleftarrow{W}_{r+1} = \begin{bmatrix} Q_{r+1} & & \\ a_{r+1}^{r+1} S_{r+1} & Q_{r+1} & \overline{F}_{r+1} \\ P_{r+1} & & \overleftarrow{M}_{r+1} \end{bmatrix} \tag{30}$$

is a core of rank $2+r \times 2+r$ and, for $r+2 \leq k \leq d-r$,

$$\overline{W}_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & \overline{F}_k \\ \overline{P}_k & & \Lambda_k \end{bmatrix} \quad \text{and} \quad \overrightarrow{W}_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & F_k \\ \overline{P}_k & & \overrightarrow{M}_k \end{bmatrix} \tag{31}$$

are cores of rank $2+r \times 2+r$ and $2+r \times 2+d-k$ respectively.

We start with the decomposition suggested by Lemma 3.2 for the value of r given by Assumption 3.4.

Reduction of the $r+1$-th rank. First, we define the cores

$$\tilde{\Theta}_{r+1} = \begin{bmatrix} \xi_1^1 & \cdots & \xi_r^1 \\ \vdots & \vdots & \vdots \\ \xi_1^{r+1} & \cdots & \xi_r^{r+1} \end{bmatrix}, \quad \overline{\Theta}_k = \begin{bmatrix} \eta_{k+1}^1 & \cdots & \eta_d^1 \\ \vdots & \vdots & \vdots \\ \eta_{k+1}^r & \cdots & \eta_d^r \end{bmatrix}$$

and $\overline{T}_k = \operatorname{diag}\left[1, 1, \overline{\Theta}_k\right]$ of rank $r+1 \times r$, $r \times d-k$ and $2+r \times 2+d-k$ respectively, where $r+1 \leq k \leq d-r-1$. According to Assumption 3.4, $\Theta_{r+1} = \tilde{\Theta}_{r+1} \bowtie \overline{\Theta}_{r+1}$. Then, by following (23), we obtain

$$\begin{bmatrix} F_{r+1} \\ M_{r+1} \end{bmatrix} = \begin{bmatrix} & X_{r+1} \\ \Sigma_{r+1} & \end{bmatrix} \bowtie \Theta_{r+1} = \begin{bmatrix} \overline{F}_{r+1} \\ \overleftarrow{M}_{r+1} \end{bmatrix} \bowtie \overline{\Theta}_{r+1},$$

where we use the relations $\overline{F}_k = \begin{bmatrix} & X_k \end{bmatrix} \bowtie \tilde{\Theta}_k$ and $\overleftarrow{M}_k = \begin{bmatrix} \\ \Sigma_k \end{bmatrix} \bowtie \tilde{\Theta}_k$. Therefore we have

$$W_{r+1} = \overleftarrow{W}_{r+1} \bowtie \overline{T}_{r+1}. \tag{32}$$

Direct sweep from $r+1$ to $d-r$. Similarly to (22), for $r+2 \leq k \leq d-r$ we may write

$$\overline{T}_{k-1} \bowtie V_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & F_k \\ \overline{P}_k & & \overrightarrow{M}_k \end{bmatrix} = \overrightarrow{W}_k, \tag{33}$$

since $\overline{\Theta}_{k-1} \bowtie \begin{bmatrix} Y_k \\ \\ \end{bmatrix} = \overline{P}_k$ and $\overline{\Theta}_{k-1} \bowtie \begin{bmatrix} \\ \Omega_k \end{bmatrix} = \overrightarrow{M}_k$. Let us note now that, similarly to (23),

$$\begin{bmatrix} F_k \\ \overrightarrow{M}_k \end{bmatrix} = \begin{bmatrix} a_{k+1}^k X_k & \cdots & a_d^k X_k \\ \eta_{k+1}^1 Q_k & \cdots & \eta_d^1 Q_{k+1} \\ \vdots & \vdots & \vdots \\ \eta_{k+1}^r Q_k & \cdots & \eta_d^r Q_{k+1} \end{bmatrix} = \begin{bmatrix} & X_k \\ \Lambda_k & \end{bmatrix} \bowtie \begin{bmatrix} \eta_{k+1}^1 & \cdots & \eta_d^1 \\ \vdots & \vdots & \vdots \\ \eta_{k+1}^r & \cdots & \eta_d^r \\ a_{k+1}^k & \cdots & a_d^k \end{bmatrix}.$$

The rank in the latter core product can be reduced: indeed, by Assumption 3.4, we have

$$\begin{bmatrix} \eta_{k+1}^1 & \cdots & \eta_d^1 \\ \vdots & \vdots & \vdots \\ \eta_{k+1}^r & \cdots & \eta_d^r \\ a_{k+1}^k & \cdots & a_d^k \end{bmatrix} = \begin{bmatrix} 1 & & \\ & \ddots & \\ & & 1 \\ \xi_1^k & \cdots & \xi_r^k \end{bmatrix} \bowtie \begin{bmatrix} \eta_{k+1}^1 & \cdots & \eta_d^1 \\ \vdots & \vdots & \vdots \\ \eta_{k+1}^r & \cdots & \eta_d^r \end{bmatrix}, \tag{34}$$

therefore $\begin{bmatrix} F_k \\ \overrightarrow{M}_k \end{bmatrix} = \begin{bmatrix} \overline{F}_k \\ \Lambda_k \end{bmatrix} \bowtie \overline{\Theta}_k$. Thus,

$$\overrightarrow{W}_k = \overline{W}_k \bowtie \overline{T}_k \tag{35}$$

for $r+2 \leq k \leq d-r-2$. Finally, (32) and the successive application of the relations (33) and (35) complete the proof. $\square$

Corollary 3.6. *Assume that $d \geq 5$, A is symmetric and, for some $\omega \in \mathbb{R}$, $Y_k = \omega X_k$ for $1 \leq k \leq d$ in (1). Let Assumption 3.4 hold true with $\zeta_p^\alpha = \xi_\alpha^p$ and $\chi_\alpha^q = \eta_q^\alpha$ for $1 \leq p < q \leq d$ and $1 \leq \alpha \leq r$. Then the following TT representation holds true:*

$$\begin{aligned} \begin{bmatrix} \mathbf{Q}_d \\ \mathbf{S}_d \end{bmatrix} &= U_1 \bowtie U_2 \bowtie \ldots \bowtie U_r \bowtie \overleftarrow{W}_{r+1} \bowtie \overline{W}_{r+2} \\ &\quad \bowtie \ldots \bowtie \overline{W}_{d-r-1} \bowtie \overrightarrow{W}_{d-r} \bowtie V_{d-r+1} \bowtie \ldots \bowtie V_{d-1} \bowtie V_d, \end{aligned}$$

where the TT ranks are $3, 4, \ldots, 2+r, \ \ldots \ , 2+r, \ldots, 4, 3$. The cores involved are the following: U_k and V_k are the same as in Corollary 3.3,

$$\overleftarrow{W}_{r+1} = \begin{bmatrix} Q_{r+1} & & \\ a_{r+1}^{r+1} S_{r+1} & Q_{r+1} & 2\omega \overline{F}_{r+1} \\ 2\omega R_{r+1} & & 2\omega \overleftarrow{M}_{r+1} \end{bmatrix},$$

is a core of rank $2+r \times 2+r$ and, for $r+2 \leq k \leq d-r$,

$$\overline{W}_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & 2\omega \overline{F}_k \\ \overline{R}_k & & \Lambda_k \end{bmatrix} \quad \text{and} \quad \overrightarrow{W}_k = \begin{bmatrix} Q_k & & \\ a_k^k S_k & Q_k & 2\omega F_k \\ 2\omega \overline{R}_k & & \overrightarrow{M}_k \end{bmatrix}$$

are of rank $2+r \times 2+r$ and $2+r \times 2+d-k$ respectively.

Proof. Follows from Lemma 3.5 in the very same way as Corollary 3.3 from Lemma 3.2. □

Note that Assumption 3.4 required by Lemma 3.5, which implies the semiseparability of A, can be substantially relaxed: actually, in the proof of Lemma 3.5 we need only that all the submatrices

$$B_k = \begin{pmatrix} a^1_{k+1} & \cdots & a^1_d \\ \vdots & \vdots & \vdots \\ a^k_{k+1} & \cdots & a^k_d \end{pmatrix} \quad \text{and} \quad C_k = \begin{pmatrix} a^{k+1}_1 & \cdots & a^d_1 \\ \vdots & \vdots & \vdots \\ a^{k+1}_k & \cdots & a^d_k \end{pmatrix} \tag{36}$$

of the strictly upper and lower triangular parts of A are of rank not greater than r. This condition is well-known in the theory of quasi-separable matrices (see, e. g., [9]) and means that the matrix A is *quasi-separable of order* r.

Once for $1 \leq k \leq d-1$ there exist a rank-r_k representation of B_k and a rank-s_k representation of C_k, it is possible to construct an explicit TT decomposition, similar to the one suggested by Lemma 3.5, of the TT ranks $2+r_1+s_1, \ldots, 2+r_{d-1}+s_{d-1}$. The technique remains the same for this generalization, the only difference is that Assumption 3.4 required by Lemma 3.5 provides a common basis for the low-rank representation of all matrices B_k, $1 \leq k \leq d-1$, and similarly for C_k. In particular, this is the reason why we have the identity subcore in (34). However, if A is only quasi-separable, it is not the case: the equation analogous to (34) contains a non-diagonal subcore accounting for the relation between the bases of low-rank representations of B_{k-1} and B_k. This results in non-diagonal subcores (composed of Q_k) instead of diagonal Λ_k in every middle core $\overline{W}_k$. This leads us to the following theorem relating the order of quasi-separability of A and the TT ranks of $\mathbf{S}_d$. The proof is similar and likewise constructive, so that the corresponding decompositions can be obtained explicitly in the same way as under Assumption 3.4 in Lemma 3.5 and Corollary 3.6 with some extra technical calculations.

Theorem 3.7. *Let* $\operatorname{rank} B_k = r_k$ *and* $\operatorname{rank} C_k = s_k$ *for* $1 \leq k \leq d-1$*, where* B_k *and* C_k *are submatrices of* A*, defined by* (36)*. Then the stiffness matrix* $\mathbf{S}_d$ *defined by* (1) *has a TT decomposition of ranks* $2+r_1+s_1, \ldots, 2+r_{d-1}+s_{d-1}$ *in terms of the diagonal of the diffusion tensor* A*, factors of corresponding rank-*r_k *and rank-*s_k *decompositions of* B_k *and* C_k *respectively, and coordinate factors* Q_k*,* S_k*,* X_k*,* Y_k*.*

If we assume additionally that A *is symmetric and, for some* $\omega \in \mathbb{R}$*,* $Y_k = \omega X_k$ *for* $1 \leq k \leq d$*, then* $\mathbf{S}_d$ *admits such a decomposition of ranks* $2+r_1, \ldots, 2+r_{d-1}$*.*

To verify the sharpness of the rank estimates obtained in Section 2.1 above, we used the *TT Toolbox* (publicly available at `http://spring.inm.ras.ru/osel`). We verified numerically that the TT decompositions given by Proposition 3.1, Lemma 3.2, Corollary 3.3 are of the smallest possible ranks for arbitrary coordinate factors Q_k, S_k, X_k and Y_k, $1 \leq k \leq d$, and the scaling factor A of the diffusion tensor. The same holds for Lemma 3.5 and Corollary 3.6, provided that additionally r in Assumption 3.4 is the exact rank of both strictly triangular parts of A. The more general estimates of the minimal TT ranks of $\mathbf{S}_d$ given in Theorem 3.7 also prove numerically to be sharp.

4 Low-rank QTT structure of the diffusion operator

In Section 3 we studied the TT structure of the matrix $\mathbf{S}_d$ defined in (1). This structure is related to the separation of d "physical" dimensions and the representation of the matrix in terms of its coordinate factors. In this section we consider $\mathbf{S}_d$ after "quantization" (see Section 2.4). We outline how, similarly to [7, Lemma 5.2], the results on the TT structure of $\mathbf{S}_d$, obtained above, lead to similar conclusions on its QTT structure, provided that the coordinate factors themselves possess a low-rank QTT structure.

Let us focus on the k-th "physical" dimension for some $1 \le k \le d$ and consider the core U_k defined in (15). From now on, when possible, we omit the index k for the sake of brevity. Let us assume that coordinate factor Q is given in a QTT representation $Q = Q^1 \bowtie Q^2 \bowtie \ldots \bowtie Q^{l-1} \bowtie Q^l$, where the QTT ranks are $\rho_Q^1, \ldots, \rho_Q^{l-1}$, and so are S, X and Y. Let us define a core $P^1 = \begin{bmatrix} a_k^1 Y^1 \\ \vdots \\ a_k^{k-1} Y^1 \end{bmatrix}$ of rank $k-1 \times \rho_Y^1$. Then for the core P of rank $k-1 \times 1$ we may write a QTT decomposition $P = P^1 \bowtie Y^2 \bowtie \ldots \bowtie Y^{l-1} \bowtie Y^l$ of ranks $\mathbf{k-1}, \rho_Y^1, \ldots, \rho_Y^{l-1}, \mathbf{1}$ (we emphasize in boldface the TT ranks, i. e. the ranks of the separation of "physical" dimensions, and do not omit the terminal ranks equal to 1). Similarly, the core Σ of rank $k-1 \times k-1$ can be represented in the QTT format as $\Sigma = \Sigma^1 \bowtie \Sigma^2 \bowtie \ldots \bowtie \Sigma^{l-1} \bowtie \Sigma^l$ with ranks $\mathbf{k-1}, (k-1)\rho_Q^1, \ldots, (k-1)\rho_Q^{l-1}, \mathbf{k-1}$ through $\Sigma^m = \operatorname{diag}[Q^m, \ldots, Q^m]$, $1 \le m \le l$.

Then for the core U of rank $2+k-1 \times 2+k$ we may write the representation $U = U^1 \bowtie U^2 \bowtie \ldots \bowtie U^{l-1} \bowtie U^l$ with the following QTT cores:

$$U^1 = \begin{bmatrix} Q^1 & & & & & \\ & a_k^k S^1 & & Q^1 & & X^1 \\ & & P^1 & & \Sigma^1 & \end{bmatrix},$$

$$U^l = \begin{bmatrix} Q^l & & & \\ S^l & & & \\ Y^l & & & \\ & Q^l & & \\ & & \Sigma^l & \\ & & & X^l \end{bmatrix} \quad \text{and} \quad U^m = \begin{bmatrix} Q^m & & & & & \\ & S^m & & & & \\ & & Y^m & & & \\ & & & Q^m & & \\ & & & & \Sigma^m & \\ & & & & & X^m \end{bmatrix}$$

for $2 \le m \le l-1$. The ranks of this QTT representation are $\mathbf{2+k-1}$, $r_U^1, \ldots, r_U^{l-1}, \mathbf{2+k}$ with $r_U^m = \rho_Q^m + \rho_S^m + \rho_Y^m + \rho_Q^m + (k-1)\rho_Q^m + \rho_X^m$ for $1 \le m \le l$.

If ρ_Q^m, ρ_S^m, ρ_X^m, ρ_Y^m are bounded from above by ρ for all $m = 1, \ldots, l$, then $r_U^m \le (k+4)\rho$. Similarly, for the cores $V = V_k$ and $W = W_k$ QTT decompositions of ranks bounded by $r_V^m \le (d-k+5)\rho$ and $r_W^m \le (\max\{k-1, d-k\} + 5)\rho$ respectively can be constructed. Then the ranks of the decomposition given by (15) with $r = \lfloor \frac{d}{2} \rfloor$ are bounded from above by $\left(\lfloor \frac{d}{2} \rfloor + 4\right)\rho = \mathcal{O}(d\rho)$. Generally, the TT decompositions obtained in Section 4 with ranks bounded by $\mathcal{O}(d)$ and $\mathcal{O}(r)$ give rise to corresponding QTT decompositions of ranks bounded by $\mathcal{O}(d\rho)$ and $\mathcal{O}(r\rho)$.

Theorem 4.1. *Assume that in* (1) *all coordinate factors S_k, Q_k, X_k and Y_k, $1 \le k \le d$, can be represented in the QTT format with ranks bounded from above by ρ. Then the matrix $\mathbf{S}_d$ defined in* (1) *can be represented in the QTT format with ranks bounded from above by:*

(a) $\left(2\lfloor \frac{d}{2} \rfloor + 7\right)\rho$*;*

(b) $(2r+7)\rho$*, if A is quasi-separable of order r;*

(c) $\left(\lfloor \frac{d}{2} \rfloor + 5\right)\rho$*, if A is triangular* or *if A is symmetric and, for some $\omega \in \mathbb{R}$, $Y_k = \omega X_k$ for $1 \le k \le d$;*

(d) $(r+5)\rho$*, if A is quasi-separable of order r and triangular* or *if A is quasi-separable of order r and symmetric and, for some $\omega \in \mathbb{R}$, $Y_k = \omega X_k$ for $1 \le k \le d$.*

In every particular case the corresponding explicit QTT decomposition and the exact expression for an upper bound on each of its ranks can be obtained as we described in this section.

Remark 4.2. *Assume that the diffusion tensor is constant, i. e. $\mathcal{K} = A$, and the standard "hat" functions are used to construct the finite element subspace. Then, according to [7, Lemma 3.1], the main assumption of Theorem 4.1 holds with $\rho = 3$.*

5 Conclusion

Above we have analyzed explicitly the TT and QTT structure of the matrices of the form (1). The efficient numerical solution of problems with anisotropic, possibly non-homogeneous diffusion (2) requires the low-rank representation of the corresponding stiffness matrix. Therefore the results of Section 2.1 and Section 2.4 contribute to the mathematical foundation of the TT- and QTT-based approaches to such problems. The localization to a hypercube is typical for financial market models, see, e. g. [31, Theorem 4.14] and [10].

Note that Lemma 3.2 proves the observation made in [5, Section 7.3 and Table 7.2], the rank estimate discussed in [6, Section 3.1] and the conjecture of [30, Hypothesis 4.9, 1.]

As we mentioned in Introduction, we consider important the relation between the quasi-separable structure of A and the TT and QTT structure of $\mathbf{S}_d$, established in Theorem 3.7 and Theorem 4.1 (b,d) respectively. In [10] so-called "ε-aggregation" was used to reduce the dimensionality of a high-dimensional diffusion model, and the corresponding error estimates were obtained [10, Theorem 2.3]. In that paper it is assumed that for some $\varepsilon \ll 1$ only $r \ll d$ eigenvalues of the rescaled volatility covariance matrix (i. e. the diffusion tensor) exceed the ε-threshold, then the d-dimensional dynamics appears to be mainly driven by r ε-aggregate diffusion processes. The diffusion tensor is approximated with rank r, and the corresponding Kolmogorov PDE was shown to reduce from d to r dimensions.

In the present paper we propose, in some sense, to reduce the *effective dimension* of discretized diffusion problems $\mathcal{L}u = f$ by considering them in the TT or QTT format. Our result affirms such a reduction to be possible under a milder condition: diffusion tensor is kept full-rank, but is assumed to have, exactly or approximately, only low-rank submatrices in the off-diagonal part. The exploration of this in the context of [10] is the subject of ongoing research.

The conclusions of the paper can be trivially generalized to linear elliptic second-order differential operators: a convection term, under an assumption on the convection coefficient, analogous to (4), has a Laplace-like structure similar to (12) and can be represented in the TT format with the help of Proposition 3.1. Then its QTT decomposition can be constructed as it is done for the diffusion operator in Section 4. The reaction term inherits the TT and QTT structure immediately from the reaction coefficient.

The assumption of the rank-1 separability of the diffusion tensor can be relaxed: we may consider diffusion tensors represented with moderate ranks in the (functional) TT format (see [32]), i. e. satisfying (3) with "$\bowtie$" instead of "$\otimes$" and the TT cores of the form (4). Equation (1) and all our proofs and conclusions can be generalized to this case by formally replacing "$\otimes$" with "$\bowtie$" and scaling all the rank estimates by the factors of the corresponding (functional) TT ranks of the diffusion tensor.

Let us also note that the results on the TT and QTT structure can be applied straightforwardly to the Hierarchical Tensor representation by Hackbusch and Kühn (see [19, 20]) with degenerate trees and its tensorized version [33], the counterpart of QTT.

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