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by

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Abstract

Ranks and explicit structure of some matrices in the Quantics Tensor Train format, which allows representation with logarithmic complexity in many cases, are investigated. The matrices under consideration are Laplace operator with various boundary conditions in D dimensions and inverse Laplace operator with Dirichlet and Dirichlet-Neumann boundary conditions in one dimension. The minimal-rank explicit QTT representations of these matrices presented are suitable for any high mode sizes and, in the multi-dimensional case, for any high dimensions.

Keywords: tensor decompositions, tensor rank, low-rank approximation, Tensor Train, TT, Quantics Tensor Train, QTT, virtual levels, tensorization, inverse Laplace operator.
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Introduction

Recent surveys on tensor methods in scientific computing [11] and data analysis [16, 5, 2] propose these methods as a mainstream means of computation in high dimensions, yielding a way to overcome the so-called "curse of dimensionality" [1]. These papers present plenty of various formats for tensor data, *canonical decomposition* and *Tucker decomposition* being the most time-honoured ones. Unfortunatelly, these two decompositions alleviate computations in high dimensions in a way rather than break the "curse of dimensionality".

We focus on a more recent format introduced in the community of numerical mathematics in 2009 by Oseledets and Tyrtyshnikov in [24] and referred to as

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Tensor Train (TT). This format makes possible to tackle high dimensions in a much more general case than the two ones mentioned above do. On the one hand, it provides the scaling of storage costs and complexity, that is linear in respect of dimensionality and linear or even sublinear (*Quantics Tensor Train*, QTT) in respect of number of points along a dimension. And, on the other hand, this format comes with robust algorithms of structured data handling [22].

In this paper we aim to present low-rank QTT structure of such the important matrices as Laplace operator in both one-dimensional and D-dimensional cases; and its inverse, in one-dimensional case. But we also have a secondary goal that is to highlight convenience and terseness of TT and contribute to a graphic comprehension of how it works.

Tensors. Canonical and Tucker decompositions

In fact, this is just a multiway array what we mean by a *tensor*. Such the objects arise naturally in discrete data analysis or after discretization of equations in scientific computing and could be recognized as arrays of coefficients of multilinear forms in some fixed basis. We refer to some tensor formats for a vector $\boldsymbol{A}(i_1, \ldots, i_D)$ of a discretized D-dimensional space below keeping in mind that a linear operator $\boldsymbol{A}(i_1, j_1, \ldots, i_D, j_D)$ over such a space can be represented in these formats just the same way, terms of decompositions having extra mode indices: another mode index j_k along with each mode index i_k, $k = 1 \ldots D$.

Once it holds for a D-dimensional $n_1 \times \ldots \times n_D$-tensor $\boldsymbol{A}$ that

$$\boldsymbol{A}(i_1, \ldots, i_D) \;=\; \sum_{\alpha=1}^{r} U_1(i_1, \alpha)\, U_2(i_2, \alpha) \cdot \ldots \cdot U_{D-1}(i_{D-1}, \alpha)\, U_D(i_D, \alpha)$$

for all the values of indices $i_k = 1 \ldots n_k$, $k = 1 \ldots D$, the tensor $\boldsymbol{A}$ is said to have a rank-r *canonical decomposition* given by the matrices $U_K \in \mathbb{R}^{n_k \times r}$, $k = 1 \ldots D$. Note that in canonical decomposition the terms U_K are tied globally throughout the product by the only rank index α. This makes the decomposition much more restrictive than, for instance, *Tucker decomposition* written as

$$\begin{aligned}\boldsymbol{A}(i_1, \ldots, i_D) \;=\; & \sum_{\alpha_1=1}^{r_1} \ldots \sum_{\alpha_D=1}^{r_D} \boldsymbol{C}(\alpha_1, \ldots, \alpha_D) \\ \cdot\; & U_1(i_1, \alpha_1)\, U_2(i_2, \alpha_2) \cdot \ldots \cdot U_{D-1}(i_{D-1}, \alpha_{D-1})\, U_D(i_D, \alpha_D),\end{aligned}$$

$\boldsymbol{C}$ being a *Tucker core* and each matrix $U_K \in \mathbb{R}^{n_k \times r_k}$, $k = 1 \ldots D$, being a *k-th mode Tucker basis*. This decomposition links the matrices U_K via the Tucker core $\boldsymbol{C}$ only, summation being performed by a single rank index α_k for each of them.

Tensor Train

Tensor $\boldsymbol{A}$ is said to be represented in the *Tensor Train* [22] format 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 it holds for all the values of indices $i_k = 1 \ldots n_k$, $k = 1 \ldots D$, that

$$\boldsymbol{A}(i_1, \ldots, i_D) \;=\; \sum_{\alpha_1=1}^{r_1} \ldots \sum_{\alpha_{D-1}=1}^{r_{D-1}} U_1(i_1, \alpha_1)\, U_2(\alpha_1, i_2, \alpha_2) \cdot \ldots \cdot$$

$$\cdot \quad U_{D-1}\left(\alpha_{D-2}, i_{D-1}, \alpha_{D-1}\right) U_D\left(\alpha_{D-1}, i_D\right). \quad (1)$$

It is plain to see that the cores are linked each to other subsequently forming a linear structure just like cars of a train, which accounts for the name TT. The summation limits $r_1 \ldots r_{D-1}$ are referred to as ranks of the tensor train.

As we mentioned above, such a representation may be applied to an operator $\boldsymbol{A}$ over a vector space as well as to a vector from it, which could be recognized as a “matricization“ of TT-cores of a “vectorized“ matrix, e. g.

$$\begin{aligned}\boldsymbol{A}\left(i_1, j_1, \ldots, i_D, j_D\right) &= \sum_{\alpha_1=1}^{r_1} \ldots \sum_{\alpha_{D-1}=1}^{r_{D-1}} U_1\left(i_1, j_1, \alpha_1\right) U_2\left(\alpha_1, i_2, j_2, \alpha_2\right) \cdot \ldots \cdot \\ &\cdot \quad U_{D-1}\left(\alpha_{D-2}, i_{D-1}, j_{D-1}, \alpha_{D-1}\right) U_D\left(\alpha_{D-1}, i_D, j_D\right). \quad (2)\end{aligned}$$

Tensor Train format was proposed by Oseledets and Tyrtyshnikov in 2009 [21, 20, 24]. It is beneficial in many aspects. First, it is based on SVD so that the problem of approximation of a tensor in this format is well-posed and robust algorithms of quasi-optimal both best rank-r approximation and ϵ-approximation are available, while this is not the case for canonical decompositon [3, 9]. Second, unlike the Tucker format, storage costs and computation complexity are linear with respect to dimensionality. Third, unlike to quite similar to the Hierarchical Tensor Format introduced in [8], TT keeps its “linear structure” throughout computations [22], which makes the algorithms in this format easier to derive, implement and understand. Further details on TT can be found in the papers [22, 24, 25, 23]; a review of tensor formats including TT is presented in [11].

Further tensorization. Quantics Tensor Train

The next step is made on the way towards efficient tensor computations is futher “tensorization“ of tensors to higher-dimensional representation by quantics-type folding [19, 10]. For any index i varied from 1 to 2^d we consider its binary representation $i = 1 + \sum_{k=1}^{d} 2^{d-k}\left(i_k - 1\right)$, each of the subindices $i_1 \ldots i_d$ being equal to either 1 or 2. These subindices compose a new multi-index $\boldsymbol{i} = \left(i_1 \ldots i_d\right)$, and hence a vector $\boldsymbol{A}$ indexed by the scalar index i is to be treated as a d-dimensional $2 \times \ldots \times 2$-tensor indexed by the multi-index $\boldsymbol{i}$. And similarly a D-dimensional $2^{d_1} \times \ldots \times 2^{d_D}$-tensor $\boldsymbol{A}$ subjected to such an index transformation is presented as a $\left(d_1 + \ldots + d_D\right)$-dimesional $2 \times \ldots \times 2$-tensor. In short, this is nothing more that just a reshaping into a $2 \times \ldots \times 2$-tensor, possibly rather high-dimensional.

Such an approach allows us to deal with high numbers of points along each dimension, dimensionality growing logarithmicaly in respect of them. Thus, a tensor format with storage costs and complexity linear with respect to dimensionality being employed along with such a reshaping, logarithmic scaling with respect to grid step can be the case.

The idea of virtual levels is not new at all. As early as in 2003 it was applied to analysis of canonical decompostion of asimptotically smooth functions [26], which in fact was done by bounding of ranks of TT cores (see also discussion in [10]). In view of TT it was considered deliberately in [19]. Being applied to TT, the idea of "tensorization" leads us to the *Quantics Tensor Train* (QTT) format with beneficial approximation properties of low-rank approximation, which was discovered in the paper [10] substantiating the computational background of the quantics folding. Tensorization has aslo been considered with respect to the Hierarchical Tucker format in [7].

The TT and QTT formats have been successfully applied recently to tensor-structured solution of stochastic PDEs [15, 14], elliptic PDEs [13, 4] and problems of quantum molecular dynamics [12], these examples being comparable to a Hierarchical Tucker-structured Krylov subspace solver for multi-parametric problems, introduced in [18]. So efficient QTT-structured iterative solvers, calling up the ones relying upon the preceding formats (for example, a tensor Krylov subspace method in canonical format presented in [17]) are already available.

TT rank

As follows from the basic paper on TT [24], the minimal possible k-th rank of an exact rather than approximate TT decomposition of a tensor $\boldsymbol{A}$ is nothing else than the rank of the corresponding unfolding of $\boldsymbol{A}$, that is the matrix $\boldsymbol{A}^{(k)}$ with the elements

$$\boldsymbol{A}^{(k)}\left(i_1 \dots i_k \; ; \; i_{k+1} \dots i_D\right) \quad = \quad \boldsymbol{A}(i_1 \dots i_D),$$

obtained from $\boldsymbol{A}$ by reshaping, indices $1 \dots k$ and $k+1 \dots D$ being considered as row and column indices respectively. This is referred to as the k-th TT rank of $\boldsymbol{A}$ [24].

Definition 0.1. A multi-way $n_1 \times \dots \times n_D$-vector

$$\boldsymbol{A} \in \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_D}$$

is given, its *k-th TT rank* is the rank of its unfolding $\boldsymbol{A}^{(k)}$ with the elements

$$\boldsymbol{A}^{(k)}\left(i_1 \dots i_k \; ; \; i_{k+1} \dots i_D\right) \quad = \quad \boldsymbol{A}(i_1 \dots i_D),$$

$1 \leq k \leq D-1$.

Once we apply this to a multi-way matrix rather than vector, TT decomposition of which is given by (2), we arrive at the same concept of TT rank. But, as it has been already noticed, this implies application of TT to a "vectorization" of the matrix. In fact, a matrix is considered merely as a *vector* in (2), and its neither possibility to map vectors to vectors nor related properties are taken into consideration. To emphasize this, we refer to this ranks as *vector TT ranks*.

Definition 0.2. A multi-way $m_1 \times n_1 \times \dots \times m_D \times n_D$-matrix

$$\boldsymbol{A} : \mathbb{R}^{n_1} \times \dots \times \mathbb{R}^{n_D} \mapsto \mathbb{R}^{m_1} \times \dots \times \mathbb{R}^{m_D}$$

is given, its *k-th vector TT rank* is the rank of its unfolding $\boldsymbol{A}^{(k)}$ with the elements

$$\boldsymbol{A}^{(k)}\left(i_1 j_1 \dots i_k j_k \; ; \; i_{k+1} j_{k+1} \dots i_D j_D\right) \quad = \quad \boldsymbol{A}(i_1 j_1 \dots i_D j_D),$$

$1 \leq k \leq D-1$.

In particular this means that the minimal vector ranks of TT decomposition of a certain matrix are somewhat independent from one other, depending on the matrix in the aggregate. So we may consider a minimal rank decomposition, which it holds for that no one of $D-1$ ranks can be reduced without introducing an error in (2) even if we allow the others to grow. And the same holds even for a decomposition with non-minimal ranks as soon as it is *orthogonal* [22]. Anyway, with no regard to if orthogonality of a decomposition holds or not, this makes it reasonable to compare ranks elementwise.

Definition 0.3. Let us say that a multiway matrix (vector) is of rank not greater than $r_1 \dots r_{D-1}$ if and only if for any k: $1 \le k \le D-1$ its k-th vector TT rank is not greater than r_k.

Vector TT rank of a matrix is of great importance in view of storage costs and complexity of such basic operations as dot product, multi-dimensional contraction, matrix-by-vector multiplication, rank reduction and orthoganalization of a tensor train. Their complexity upper bounds are linear with respect to vector TT rank upper bound raised to the power 2 or 3 [22].

Operators to be considered

In this paper we focus on QTT structure of finite difference discretization $\mathbf{\Delta}^{(d_1 \dots d_D)}$ of Laplace operator, considered over a D-dimensional cube on tensor uniform grids, and, in one-dimensional case, of its inverse as well. The grids in question are tensor products of D one-dimensional uniform grids, each k-th of them comprising 2^{d_k} points. Specifically, by discrete Laplace operator we mean a matrix

$$\mathbf{\Delta}^{(d_1 \dots d_D)} = a_1 \mathbf{\Delta}_1^{(d_1)} \otimes \mathbb{I}_{2^{d_2}} \dots \otimes \mathbb{I}_{2^{d_D}} + \dots + \mathbb{I}_{2^{d_1}} \otimes \dots \otimes \mathbb{I}_{2^{d_{D-1}}} \otimes a_D \mathbf{\Delta}_D^{(d_D)}, \tag{3}$$

summed by D terms here, $\mathbb{I}_m$ being an $m \times m$ identity matrix. The weights a_k are to take into consideration both the difference in grid steps and anisotropy. For the sake of brevity these weights are let be 1 below unless otherwise stated. Each of $\mathbf{\Delta}_k^{(d_k)}$ may be any of the following $2^{d_k} \times 2^{d_k}$-matrices, depending on the boundary conditions imposed:

$$\mathbf{\Delta}_{DD}^{(d_k)} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}, \quad \mathbf{\Delta}_{NN}^{(d_k)} = \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix} \tag{4}$$

are the ones for Dirichlet and Neumann boundary conditions respectively,

$$\mathbf{\Delta}_{DN}^{(d_k)} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}, \quad \mathbf{\Delta}_{ND}^{(d_k)} = \begin{pmatrix} 1 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \tag{5}$$

are the ones for various boundary conditions in the two boundary points and

$$\mathbf{\Delta}_P^{(d_k)} = \begin{pmatrix} 2 & -1 & & & -1 \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ -1 & & & -1 & 2 \end{pmatrix} \tag{6}$$

is the one for periodic boundary conditions.

Notation

QTT structure of the operators described above and some other related ones is to be revealed in terms of the following 2×2-matrices:

$$I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad J = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad I_1 = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad I_2 = \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}, \quad P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

$$E = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad F = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad K = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{7}$$

To deal with 3 and 4-dimensional TT cores efficiently in the paper, we use matrix notation for them and their convolutions a lot. For instance, if $n \times m$-matrices $A_{\alpha\beta}$, $\alpha = 1 \ldots r_1$, $\beta = 1 \ldots r_2$ are the TT blocks of a TT core U of mode sizes n and m, left rank r_1 and right rank r_2, so that $U(\alpha, i, j, \beta) = (A_{\alpha\beta})_{ij}$ for all the values of the indices, then we write it just as a matrix

$$U = \begin{bmatrix} A_{11} & \cdots & A_{1r_2} \\ \vdots & \vdots & \vdots \\ A_{r_1 1} & \cdots & A_{r_1 r_2} \end{bmatrix},$$

a *core matrix*, in square braces. As long as we aim to present TT structure in terms of a narrow set of TT blocks, we need to focus on rank structure of the cores, and that is why such a notation is convenient in handling the cores of TT decomposition.

Definition 0.4. For two TT cores U and V of sizes $p \times n \times m \times q$ and $q \times k \times l \times r$ respectively, consisting of TT blocks $A_{\alpha\gamma}$, $\alpha = 1 \ldots p$, $\gamma = 1 \ldots q$ and $B_{\gamma\beta}$, $\gamma = 1 \ldots q$, $\beta = 1 \ldots r$ respectively, let us define their *inner core product* $U \bowtie V$ as a TT core of size $p \times nk \times ml \times r$, comprising TT blocks $\sum_{\gamma=1}^{q} A_{\alpha\gamma} \otimes B_{\gamma\beta}$, $\alpha = 1 \ldots p$, $\beta = 1 \ldots r$.

In other words, we define $U \bowtie V$ as a regular matrix product of the two core matrices, their elements (TT blocks) being multiplied by means of tensor product. For example,

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

Definition 0.5. For two TT cores U and V of sizes $p \times n \times k \times q$ and $r \times k \times m \times s$ respectively, consisting of TT blocks $A_{\alpha\beta}$, $\alpha = 1 \dots p$, $\beta = 1 \dots q$ and $B_{\alpha\beta}$, $\alpha = 1 \dots r$, $\beta = 1 \dots s$ respectively, let us define their *outer core product* $U \bullet V$ as a TT core of size $pr \times n \times m \times qs$, comprising TT blocks $A_{\alpha\beta} \cdot B_{\gamma\delta}$, $\alpha = 1 \dots p$, $\beta = 1 \dots q$, $\gamma = 1 \dots r$, $\delta = 1 \dots s$.

The latter operation is very similar to the former one, regular matrix and tensor multiplications being interchanged. For instance,

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} \bullet \begin{bmatrix} B_{11} & B_{12} \\ B_{21} & B_{22} \end{bmatrix} = \begin{bmatrix} A_{11}B_{11} & A_{11}B_{12} & A_{12}B_{11} & A_{12}B_{12} \\ A_{11}B_{21} & A_{11}B_{22} & A_{12}B_{21} & A_{12}B_{22} \\ A_{21}B_{11} & A_{21}B_{12} & A_{22}B_{11} & A_{22}B_{12} \\ A_{21}B_{21} & A_{21}B_{22} & A_{22}B_{21} & A_{22}B_{22} \end{bmatrix}.$$

In order to avoid confusion we use square braces for TT cores, which are to be multiplied by means of inner or outer core product, and round braces for regular matrices, which are to be multiplied as usual.

Remark 0.6. Both core products introduced above arise naturally from the TT format. For instance, (2) could be recast as

$$\boldsymbol{A} = U_1 \bowtie U_2 \bowtie \dots \bowtie U_{D-1} \bowtie U_D.$$

Let $\boldsymbol{B} = V_1 \bowtie V_2 \bowtie \dots \bowtie V_{D-1} \bowtie V_D$, then a linear combination of $\boldsymbol{A}$ and $\boldsymbol{B}$ could be put down as following:

$$\alpha \boldsymbol{A} + \beta \boldsymbol{B} = \begin{bmatrix} U_1 & \big| & V_1 \end{bmatrix} \bowtie \left[\begin{array}{c|c} U_2 & \\ \hline & V_2 \end{array}\right] \bowtie \dots \bowtie \left[\begin{array}{c|c} U_{D-1} & \\ \hline & V_{D-1} \end{array}\right] \bowtie \left[\begin{array}{c} \alpha U_D \\ \hline \beta V_D \end{array}\right];$$

a tensor product of $\boldsymbol{A}$ and $\boldsymbol{B}$, as following:

$$\boldsymbol{A} \otimes \boldsymbol{B} = U_1 \bowtie U_2 \bowtie \dots \bowtie U_{D-1} \bowtie U_D \bowtie V_1 \bowtie V_2 \bowtie \dots \bowtie V_{D-1} \bowtie V_D;$$

a matrix product of $\boldsymbol{A}$ and $\boldsymbol{B}$, as following:

$$\boldsymbol{AB} = (U_1 \bullet V_1) \bowtie (U_2 \bullet V_2) \bowtie \dots \bowtie (U_{D-1} \bullet V_{D-1}) \bowtie (U_D \bullet V_D).$$

It is also plain to see that a transpose $\boldsymbol{A}'$ of $\boldsymbol{A}$ is equal to an inner core product of the same TT cores, their TT blocks being transposed.

Finally, by $A^{\otimes k}$, k being natural, we mean a k-th tensor power of A. For example, $I^{\otimes 3} = I \otimes I \otimes I$, and the same way for the core product operations "$\bowtie$" and "$\bullet$".

1 Some examples of derivation TT and QTT structure

Next we will derive TT and QTT decompositions of some matrices to manifest the notation introduced above, bring into play our basic technique allowing us to do the same job with the other matrices under consideration and prepare important preliminaries. In fact, the idea is very simple. We apply two sequential steps recursively. First, we pick a higher level of TT structure in terms of the basic TT blocks chosen. Second, we get rid of redundancy of a decomposition, which turns out to be evident thanks to a wise choice of the basic blocks.

1.1 TT structure of a "D-dimensional" Laplace-like operator

We start off with the operator 3, that was announced above to be of the most interest for us in this paper. Below we will also need a similar Laplace-like operator $\boldsymbol{\mathcal{L}}^{(D)}$, $D \geq 2$, with a slightly more general structure:

$$\begin{aligned} \boldsymbol{\mathcal{L}}^{(D)} &= M_1 \otimes R_2 \otimes R_3 \otimes \ldots \otimes R_{D-2} \otimes R_{D-1} \otimes R_D \\ &+ L_1 \otimes M_2 \otimes R_3 \otimes \ldots \otimes R_{D-2} \otimes R_{D-1} \otimes R_D + \ldots \\ &+ L_1 \otimes L_2 \otimes L_3 \otimes \ldots \otimes L_{D-2} \otimes M_{D-1} \otimes R_D \\ &+ L_1 \otimes L_2 \otimes L_3 \otimes \ldots \otimes L_{D-2} \otimes L_{D-1} \otimes M_D, \end{aligned} \tag{8}$$

matrices L_k, M_k and R_k being of size $m_k \times n_k$, $1 \leq k \leq D$.

Lemma 1.1. *For any $D \geq 2$ the Laplace-like operator $\boldsymbol{\mathcal{L}}^{(D)}$ allows the following rank-$2 \ldots 2$ TT representation in terms of the blocks L_k, M_k and R_k:*

$$\boldsymbol{\mathcal{L}}^{(D)} = \begin{bmatrix} L_1 & M_1 \end{bmatrix} \bowtie \begin{bmatrix} L_2 & M_2 \\ & R_2 \end{bmatrix} \bowtie \ldots \bowtie \begin{bmatrix} L_{D-1} & M_{D-1} \\ & R_{D-1} \end{bmatrix} \bowtie \begin{bmatrix} M_D \\ R_D \end{bmatrix}.$$

Proof. The first level of TT structure of this operator is trivially exposed right from the definition (8) given by means of canonical format. Indeed,

$$\boldsymbol{\mathcal{L}}^{(k+1)} = \boldsymbol{\mathcal{L}}^{(k)} \otimes R_{k+1} + L_1 \otimes \ldots \otimes L_k \otimes M_{k+1},$$

which holds for any $k \geq 2$ and can also be recast by means of core inner product into the following:

$$\boldsymbol{\mathcal{L}}^{(k+1)} = \begin{bmatrix} L_1 \otimes \ldots \otimes L_k & \boldsymbol{\mathcal{L}}^{(k)} \end{bmatrix} \bowtie \begin{bmatrix} M_{k+1} \\ R_{k+1} \end{bmatrix},$$

the latter, being applied to itself recusively, allows us to draw up a rank-2 TT decomposition of the "D-dimensional" operator $\boldsymbol{\mathcal{L}}^{(D)}$ in terms of "one-dimensional" operators L_k, M_k and R_k, $1 \leq k \leq D$:

$$\begin{aligned} \boldsymbol{\mathcal{L}}^{(D)} &= \begin{bmatrix} L_1 \otimes \ldots \otimes L_{D-1} & \boldsymbol{\mathcal{L}}^{(D-1)} \end{bmatrix} \bowtie \begin{bmatrix} M_D \\ R_D \end{bmatrix} \\ &= \begin{bmatrix} L_1 \otimes \ldots \otimes L_{D-2} & L_1 \otimes \ldots \otimes L_{D-2} & \boldsymbol{\mathcal{L}}^{(D-2)} \end{bmatrix} \bowtie \begin{bmatrix} L_{D-1} & \\ & M_{D-1} \\ & R_{D-1} \end{bmatrix} \bowtie \begin{bmatrix} M_D \\ R_D \end{bmatrix} \\ &= \begin{bmatrix} L_1 \otimes \ldots \otimes L_{D-2} & \boldsymbol{\mathcal{L}}^{(D-2)} \end{bmatrix} \bowtie \begin{bmatrix} L_{D-1} & M_{D-1} \\ & R_{D-1} \end{bmatrix} \bowtie \begin{bmatrix} M_D \\ R_D \end{bmatrix} = \ldots \\ &= \begin{bmatrix} L_1 \otimes L_2 & \boldsymbol{\mathcal{L}}^{(2)} \end{bmatrix} \bowtie \begin{bmatrix} L_3 & M_3 \\ & R_3 \end{bmatrix} \bowtie \ldots \bowtie \begin{bmatrix} L_{D-1} & M_{D-1} \\ & R_{D-1} \end{bmatrix} \bowtie \begin{bmatrix} M_D \\ R_D \end{bmatrix} \\ &= \begin{bmatrix} L_1 & M_1 \end{bmatrix} \bowtie \begin{bmatrix} L_2 & M_2 \\ & R_2 \end{bmatrix} \bowtie \ldots \bowtie \begin{bmatrix} L_{D-1} & M_{D-1} \\ & R_{D-1} \end{bmatrix} \bowtie \begin{bmatrix} M_D \\ R_D \end{bmatrix}. \end{aligned} \tag{9}$$

□

Remark 1.2. Once QTT decompositions of each of "one-dimensional" operators L_k, M_k and R_k, $1 \leq k \leq D$, are known, they can easily be merged into a QTT decomposition of the "D-dimensional" operator $\boldsymbol{\mathcal{L}}^{(D)}$ according to Lemma 1.1. For instance, if $L = U_1 \bowtie \ldots \bowtie U_d$, $M = V_1 \bowtie \ldots \bowtie V_d$ and $R = W_1 \bowtie \ldots \bowtie W_d$, U_k, V_k and W_k, $1 \leq k \leq d$ being QTT cores, then

$$\begin{aligned}
\begin{bmatrix} L & M \\ & R \end{bmatrix} &= \left[\begin{array}{c|c|c} U_1 & V_1 & \\ \hline & & W_1 \end{array}\right] \\
&\bowtie \left[\begin{array}{c|c|c} U_2 & & \\ \hline & V_2 & \\ \hline & & W_2 \end{array}\right] \bowtie \ldots \bowtie \left[\begin{array}{c|c|c} U_{d-1} & & \\ \hline & V_{d-1} & \\ \hline & & W_{d-1} \end{array}\right] \bowtie \left[\begin{array}{c|c} U_d & \\ \hline & V_d \\ \hline & W_d \end{array}\right], \\
\begin{bmatrix} L & M \end{bmatrix} &= \left[\begin{array}{c|c} U_1 & V_1 \end{array}\right] \bowtie \left[\begin{array}{c|c} U_2 & \\ \hline & V_2 \end{array}\right] \bowtie \ldots \bowtie \left[\begin{array}{c|c} U_{d-1} & \\ \hline & V_{d-1} \end{array}\right] \bowtie \left[\begin{array}{c|c} U_d & \\ \hline & V_d \end{array}\right], \\
\begin{bmatrix} M \\ R \end{bmatrix} &= \left[\begin{array}{c|c} V_1 & \\ \hline & W_1 \end{array}\right] \bowtie \left[\begin{array}{c|c} V_2 & \\ \hline & W_2 \end{array}\right] \bowtie \ldots \bowtie \left[\begin{array}{c|c} V_{d-1} & \\ \hline & W_{d-1} \end{array}\right] \bowtie \left[\begin{array}{c} V_d \\ \hline W_d \end{array}\right],
\end{aligned} \tag{10}$$

core product is to be applied with no respect to the extra block structure of cores marked by lines. In general case such the cores $U_1 \ldots U_d$, $V_1 \ldots V_d$ and $W_1 \ldots W_d$, that the ranks of these representations cannot be reduced, do exist. But we tackle particular L, M and R, which mostly allow us to lessen ranks of the QTT decomposition (10) of $\boldsymbol{\mathcal{L}}^{(D)}$.

Now we are prepared to proceed easily from a sum of D tensor products of rank-1 TT cores $\boldsymbol{\mathcal{L}}^{(D)}$ to a sum of D products of TT cores of arbitrary compatible ranks

$$\boldsymbol{\mathcal{M}}^{(D)} = \sum_{k=1}^{D} U_1 \bowtie \ldots \bowtie U_{k-1} \bowtie \Gamma_k \bowtie V_{k+1} \bowtie \ldots \bowtie V_D, \tag{11}$$

U_k, Γ_k and V_k, $1 \leq k \leq D$, being cores of consistent rank and mode sizes, so that each of the summands in (11) and the sum itself are correctly defined. Note that $\boldsymbol{\mathcal{M}}^{(D)}$ is a straightforward generalization of $\boldsymbol{\mathcal{L}}^{(D)}$. Indeed, (11) turns into (8) as long as $U_k = \begin{bmatrix} L_k \end{bmatrix}$, $\Gamma_k = \begin{bmatrix} M_k \end{bmatrix}$ and $V_k = \begin{bmatrix} R_k \end{bmatrix}$, $1 \leq k \leq D$.

It is to be pointed out that we do not limit $\boldsymbol{\mathcal{M}}^{(D)}$ to a sum of D "complete" tensor trains. We consider the case when the left rank of U_1 and Γ_1, as well as the right rank of Γ_D and V_D are not required to be equal to 1, and hence $\boldsymbol{\mathcal{M}}^{(D)}$ may in general depend also on two rank indices. The following statement, similar to Lemma 1.1, holds for such the structured matrix.

Lemma 1.3. *For any $D \geq 2$ the operator $\boldsymbol{\mathcal{M}}^{(D)}$ allows the following rank-$2 \ldots 2$ TT representation in terms of the cores U_k, Γ_k and V_k:*

$$\boldsymbol{\mathcal{M}}^{(D)} = \left[\begin{array}{c|c} U_1 & \Gamma_1 \end{array}\right] \bowtie \left[\begin{array}{c|c} U_2 & \Gamma_2 \\ \hline & V_2 \end{array}\right] \bowtie \ldots \bowtie \left[\begin{array}{c|c} U_{D-1} & \Gamma_{D-1} \\ \hline & V_{D-1} \end{array}\right] \bowtie \left[\begin{array}{c} \Gamma_D \\ \hline V_D \end{array}\right].$$

Proof. Follows the proof of Lemma 1.1 owing to the properties of the inner core product inherited from the matrix multiplication and tensor product, "$\otimes$" being replaced with "$\bowtie$"; L_k, M_k and R_k, with U_k, Γ_k and V_k respectively. $\square$

1.2 "One-dimensional" shift and gradient matrices

Let us now go ahead with QTT structure of the two such recognizable "one-dimensional" operators as shift and gradient matrices:

$$\boldsymbol{S}^{(d)} = \begin{pmatrix} 0 & 1 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 0 & 1 & 0 \\ & & & 0 & 1 \\ & & & & 0 \end{pmatrix} \quad \text{and} \quad \boldsymbol{G}^{(d)} = \begin{pmatrix} 1 & -1 & 0 & & \\ & \ddots & \ddots & \ddots & \\ & & 1 & -1 & 0 \\ & & & 1 & -1 \\ & & & & 1 \end{pmatrix},$$

size of both being equal 2^d. A simple recursive block structure of $\boldsymbol{G}^{(k)}$

$$\boldsymbol{G}^{(k)} = \left(\begin{array}{c|c} \boldsymbol{G}^{(k-1)} & -J'^{\otimes(k-1)} \\ \hline & \boldsymbol{G}^{(k-1)} \end{array}\right) = I \otimes \boldsymbol{G}^{(k-1)} - J \otimes J'^{\otimes(k-1)},$$

in our core product notation leads straightforwardly to

$$\begin{aligned} \boldsymbol{G}^{(d)} &= \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{G}^{(d-1)} \\ -J'^{\otimes(d-1)} \end{bmatrix} = \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} I & J & \\ & & J' \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{G}^{(d-2)} \\ -J'^{\otimes(d-2)} \\ -J'^{\otimes(d-2)} \end{bmatrix} \\ &= \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{G}^{(d-2)} \\ -J'^{\otimes(d-2)} \end{bmatrix} = \ldots = \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} \boldsymbol{G}^{(1)} \\ -J' \end{bmatrix} \\ &= \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} I - J \\ -J' \end{bmatrix}. \end{aligned} \tag{12}$$

Decomposition of a shift matrix is obtained by the same token:

$$\boldsymbol{S}^{(d)} = \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} \boldsymbol{S}^{(1)} \\ J' \end{bmatrix} = \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} J \\ J' \end{bmatrix}. \tag{13}$$

Likewise, for periodical shift and gradient matrices

$$\begin{aligned} \boldsymbol{S}_P^{(d)} &= \boldsymbol{S}^{(d)} + \begin{pmatrix} & \\ 1 & \end{pmatrix} = \boldsymbol{S}^{(d)} + \begin{bmatrix} J' \end{bmatrix}^{\bowtie d}, \\ \boldsymbol{G}_P^{(d)} &= \boldsymbol{G}^{(d)} - \begin{pmatrix} & \\ 1 & \end{pmatrix} = \boldsymbol{G}^{(d)} - \begin{bmatrix} J' \end{bmatrix}^{\bowtie d} \end{aligned}$$

it holds that

$$\begin{aligned} \boldsymbol{S}_P^{(d)} &= \begin{bmatrix} I & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J & \\ & J' & \\ & & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} J \\ J' \\ J' \end{bmatrix} \\ &= \begin{bmatrix} I & P \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} J \\ J' \end{bmatrix}, \end{aligned} \tag{14}$$

$$\begin{aligned} \boldsymbol{G}_P^{(d)} &= \begin{bmatrix} I & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J & \\ & J' & \\ & & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} I - J \\ -J' \\ -J' \end{bmatrix}. \\ &= \begin{bmatrix} I & P \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} I - J \\ -J' \end{bmatrix}. \end{aligned} \tag{15}$$

Remark 1.4. Transposition of Tensor Trains notation require no effort in core notation, all one needs to do is to transpose all the TT blocks. For instance, inverse periodical shift matrix has the following QTT representation:

$$\boldsymbol{G}_P^{(d)\prime} \quad = \quad \begin{bmatrix} I & J'+J \end{bmatrix} \bowtie \begin{bmatrix} I & J' \\ & J \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} I-J' \\ -J \end{bmatrix}.$$

Remark 1.5. As long as $\boldsymbol{\Delta}_{DN}^{(d)} = \boldsymbol{G}^{(d)} \boldsymbol{G}^{(d)\prime}$, $\boldsymbol{\Delta}_{ND}^{(d)} = \boldsymbol{G}^{(d)\prime} \boldsymbol{G}^{(d)}$ and $\boldsymbol{\Delta}_{P}^{(d)} = \boldsymbol{G}_P^{(d)} \boldsymbol{G}_P^{(d)\prime}$, we could now use (12) and (15) to derive QTT decompositions of these "one-dimensional" Laplace operators. For instance,

$$\begin{aligned}
\boldsymbol{\Delta}_P^{(d)} \quad &= \quad \left(\begin{bmatrix} I & P \end{bmatrix} \bullet \begin{bmatrix} I & P \end{bmatrix}\right) \bowtie \left(\begin{bmatrix} I & J \\ & J' \end{bmatrix} \bullet \begin{bmatrix} I & J' \\ & J \end{bmatrix} \right)^{\bowtie (d-2)} \bowtie \left(\begin{bmatrix} I-J \\ -J' \end{bmatrix} \bullet \begin{bmatrix} I-J' \\ -J \end{bmatrix} \right) \\
&= \quad \begin{bmatrix} II & IP & PI & PP \end{bmatrix} \\
&\bowtie \quad \begin{bmatrix} II & IJ' & JI & JJ' \\ & IJ & & JJ \\ & & J'I & J'J' \\ & & & J'J \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} (I-J)(I-J') \\ -(I-J)J \\ J'(I-J') \\ J'J \end{bmatrix},
\end{aligned}$$

which could be simplified to a rank-$2, 3 \dots 3$ decomposition to be obtained another way below.

2 Laplace operator

2.1 One dimension

Consider "one-dimensional" Laplace operator $\boldsymbol{\Delta}_{DD}^{(d)}$ (4). Like the gradient matrix dealt with above it has a low-rank QTT structure, as it follows from the next lemma.

Lemma 2.1. *For any $d \geq 2$ it holds that*

$$\boldsymbol{\Delta}_{DD}^{(d)} \quad = \quad \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix}.$$

Proof. Similarly to a gradient matrix, $\boldsymbol{\Delta}_{DD}^{(d)}$ exhibits a recursive block structure:

$$\boldsymbol{\Delta}_{DD}^{(k)} = \left(\begin{array}{c|c} \boldsymbol{\Delta}_{DD}^{(k-1)} & -J'^{\otimes (k-1)} \\ \hline -J^{\otimes (k-1)} & \boldsymbol{\Delta}_{DD}^{(k-1)} \end{array} \right) = I \otimes \boldsymbol{\Delta}_{DD}^{(k-1)} - J' \otimes J^{\otimes (k-1)} - J \otimes J'^{\otimes (k-1)},$$

which yields us its low-rank QTT representation:

$$\boldsymbol{\Delta}_{DD}^{(d)} \quad = \quad \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{\Delta}^{(d-1)} \\ -J^{\otimes (d-1)} \\ -J'^{\otimes (d-1)} \end{bmatrix} = \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & & & J & \\ & & & & J' \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{\Delta}^{(d-2)} \\ -J^{\otimes (d-2)} \\ -J'^{\otimes (d-2)} \\ -J^{\otimes (d-2)} \\ -J'^{\otimes (d-2)} \end{bmatrix}$$

$$= \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{\Delta}^{(d-2)} \\ -J^{\otimes(d-2)} \\ -J'^{\otimes(d-2)} \end{bmatrix} = \ldots =$$

$$= \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix}.$$

□

This lemma leads us to similar results for a discretized one-dimensional Laplace operator in case of other boundary conditions.

Lemma 2.2. *For any* $d \geq 4$ *it holds that*

$$\boldsymbol{\Delta}_{DN}^{(d)} = \begin{bmatrix} I & J' & J & I_2 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I_2 \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_2 \end{bmatrix},$$

$$\boldsymbol{\Delta}_{ND}^{(d)} = \begin{bmatrix} I & J' & J & I_1 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I_1 \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_1 \end{bmatrix},$$

$$\boldsymbol{\Delta}_{NN}^{(d)} = \begin{bmatrix} I & J' & J & I_2 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & I_1 \\ & J & & & \\ & & J' & & \\ & & & I_2 & -I_1 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & I_2 & \\ & & & & I_1 \end{bmatrix}^{\bowtie(d-4)}$$

$$\bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I_2 \\ -\frac{1}{2}I_1 & \frac{1}{2}I_1 & \frac{1}{2}I_1 & -I_1 \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_2 \end{bmatrix},$$

$$\boldsymbol{\Delta}_{P}^{(d)} = \begin{bmatrix} I & P \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie(d-3)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix}.$$

Proof. Since $\boldsymbol{\Delta}_{DN}^{(d)} = \boldsymbol{\Delta}_{DD}^{(d)} - I_2^{\otimes d}$ and $\boldsymbol{\Delta}_{ND}^{(d)} = \boldsymbol{\Delta}_{DD}^{(d)} - I_1^{\otimes d}$, we arrive at the decompositions of these operators at once in view of Lemma 2.1. In the same way, as long as $\boldsymbol{\Delta}_{NN}^{(d)} = \boldsymbol{\Delta}_{DD}^{(d)} - I_1^{\otimes d} - I_2^{\otimes d}$, it follows that

$$\boldsymbol{\Delta}_{NN}^{(d)} = \begin{bmatrix} I & J' & J & I_2 & I_1 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & I_2 & \\ & & & & I_1 \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_2 \\ -I_1 \end{bmatrix},$$

and due to the fact that $I_1 + I_2 = I$ we can reduce both the terminal ranks down to 4:

$$
\begin{aligned}
\mathbf{\Delta}_{NN}^{(d)} &= \begin{bmatrix} I & J' & J & I_2 \end{bmatrix} \bowtie \begin{bmatrix} 1 & & & 1 \\ & 1 & & \\ & & 1 & \\ & & 1 & -1 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & I_2 & \\ & & & & I_1 \end{bmatrix}^{\bowtie (d-2)} \\
&\bowtie \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & 1 & \\ & & & 1 \\ -\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & -1 \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_2 \end{bmatrix},
\end{aligned}
$$

For periodic boundary conditions, since $\mathbf{\Delta}_P^{(d)} = \mathbf{\Delta}_{DD}^{(d)} - J^{\otimes d} - J'^{\otimes d}$, we elicit the following QTT decomposition.

$$
\begin{aligned}
\mathbf{\Delta}_P^{(d)} &= \begin{bmatrix} I & J' & J & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & J & \\ & & & & J' \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -J \\ -J' \end{bmatrix} \\
&= \begin{bmatrix} I & J' & J & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & J & \\ & & & & J' \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \\ & 1 & \\ & & 1 \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix} \\
&= \begin{bmatrix} I & J' & J & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & J & \\ & & & & J' \end{bmatrix}^{\bowtie (d-3)} \bowtie \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \\ & 1 & \\ & & 1 \end{bmatrix} \\
&\bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix} \\
&= \ldots = \begin{bmatrix} I & J' & J & J & J' \end{bmatrix} \bowtie \begin{bmatrix} 1 & & \\ & 1 & \\ & & 1 \\ & 1 & \\ & & 1 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix} \\
&= \begin{bmatrix} I & P \end{bmatrix} \bowtie \begin{bmatrix} 1 & & \\ & 1 & 1 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix} \\
&= \begin{bmatrix} I & P \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie (d-3)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix},
\end{aligned}
$$

which consequently has ranks smaller or equal to those of $\mathbf{\Delta}_{DD}^{(d)}$ that we started with. □

2.2 D dimensions

As soon as $M_k = a_k \mathbf{\Delta}_k^{(d_k)}$ and $L_k = R_k = I^{\otimes d_k}$ for any $k = 1 \dots D$, $\boldsymbol{\mathcal{L}}^{(D)}$ (8) is a Laplace operator $\mathbf{\Delta}^{(d_1 \dots d_D)}$ (3), and hence the following corollary to Lemma 1.1 holds.

Corollary 2.3. *For any $D \geq 2$ the "D-dimensional" Laplace operator defined by* (3) *has the following QTT structure in terms of the "one-dimensional" Laplace operators $a_k \mathbf{\Delta}_k^{(d_k)}$, $1 \leq k \leq D$:*

$$\begin{aligned} \mathbf{\Delta}^{(d_1 \dots d_D)} &= \begin{bmatrix} I^{\otimes d_1} & a_1 \mathbf{\Delta}_1^{(d_1)} \end{bmatrix} \\ &\bowtie \begin{bmatrix} I^{\otimes d_2} & a_2 \mathbf{\Delta}_2^{(d_2)} \\ & I^{\otimes d_2} \end{bmatrix} \bowtie \dots \bowtie \begin{bmatrix} I^{\otimes d_{D-1}} & a_{D-1} \mathbf{\Delta}_{D-1}^{(d_{D-1})} \\ & I^{\otimes d_{D-1}} \end{bmatrix} \bowtie \begin{bmatrix} a_D \mathbf{\Delta}_D^{(d_D)} \\ I^{\otimes d_D} \end{bmatrix}. \end{aligned}$$

Next we match this with results of Lemma 2.1 and Lemma 2.2 according to the Remark 1.2. As soon as we derive low-rank QTT representations of the supercores involved in (10), we will have the one of the Laplace operator comprising these supercores at once.

In case of Dirichlet boundary conditions we put QTT cores into the supercores involved in (10) and do the same thing as before: reduce ranks as possible by elimination of dependent QTT blocks, which could be conceived as sweeping column (in regard to the left core) or row (in regard to the right core) transformation matrices through the "tensor train" just as it was done in the proof of Lemma 2.2. In cases of other boundary conditions QTT decompositions may be derived by the same token and the alterations to the Dirichlet boundary conditions case required are quite evident.

Corollary 2.4. *For any $d \geq 3$ the following QTT representations hold.*

$$\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_{DD}^{(d_k)} \\ & I^{\otimes d_k} \end{bmatrix} = \begin{bmatrix} I & J' & J & \\ & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} I & a_k \left(2I - J - J'\right) \\ & -a_k J \\ & -a_k J' \\ & I \end{bmatrix},$$

$$\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_{DD}^{(d_k)} \end{bmatrix} = \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} I & a_k \left(2I - J - J'\right) \\ & -a_k J \\ & -a_k J' \end{bmatrix},$$

$$\begin{aligned} \begin{bmatrix} a_k \mathbf{\Delta}_{DD}^{(d_k)} \\ I^{\otimes d_k} \end{bmatrix} &= \begin{bmatrix} I & J' & J & \\ & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I \end{bmatrix}^{\bowtie (d-3)} \\ &\bowtie \begin{bmatrix} a_k I & a_k J' & a_k J & \\ & a_k J & & \\ & & a_k J' & \\ \frac{1}{2} I & -\frac{1}{2} I & -\frac{1}{2} I & \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix}. \end{aligned}$$

Proof.

$$
\begin{aligned}
\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_{DD}^{(d_k)} \\ & I^{\otimes d_k} \end{bmatrix}
&= \begin{bmatrix} I & I & J' & J & \\ & & & & I \end{bmatrix} \\
&\bowtie \begin{bmatrix} I & & & & \\ & I & J' & J & \\ & & J & & \\ & & & J' & \\ & & & & I \end{bmatrix}^{\bowtie (d-2)}
\bowtie \begin{bmatrix} I & \\ & a_k\,(2I - J - J') \\ & -a_k J \\ & -a_k J' \\ & I \end{bmatrix} \\
&= \begin{bmatrix} I & J' & J & \\ & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I \end{bmatrix}^{\bowtie (d-2)}
\bowtie \begin{bmatrix} I & a_k\,(2I - J - J') \\ & -a_k J \\ & -a_k J' \\ & I \end{bmatrix},
\end{aligned}
$$

for a middle supercore. The terminal supercores are subcores of that, which allows to reduce ranks of them similarly to how it was done in the proof of Lemma 2.2. □

Corollary 2.5. *For any $d \geq 3$ the following QTT representations hold:*

$$
\begin{aligned}
\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_{DN}^{(d_k)} \\ & I^{\otimes d_k} \end{bmatrix}
&= \begin{bmatrix} I & J' & J & I_2 & \\ & & & & I \end{bmatrix} \\
&\bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & I_2 & \\ & & & & I \end{bmatrix}^{\bowtie (d-2)}
\bowtie \begin{bmatrix} I & a_k\,(2I - J - J') \\ & -a_k J \\ & -a_k J' \\ & -a_k I_2 \\ & I \end{bmatrix}, \\
\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_{DN}^{(d_k)} \end{bmatrix}
&= \begin{bmatrix} I & J' & J & I_2 \end{bmatrix} \\
&\bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I_2 \end{bmatrix}^{\bowtie (d-2)}
\bowtie \begin{bmatrix} I & a_k\,(2I - J - J') \\ & -a_k J \\ & -a_k J' \\ & -a_k I_2 \end{bmatrix}, \\
\begin{bmatrix} a_k \mathbf{\Delta}_{DN}^{(d_k)} \\ I^{\otimes d_k} \end{bmatrix}
&= \begin{bmatrix} I & J' & J & I_2 & \\ & & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & I_2 & \\ & & & & I \end{bmatrix}^{\bowtie (d-3)} \\
&\bowtie \begin{bmatrix} a_k I & a_k J' & a_k J & \\ & a_k J & & \\ & & a_k J' & \\ & & & a_k I_2 \\ \frac{1}{2} I & -\frac{1}{2} I & -\frac{1}{2} I & \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_2 \end{bmatrix},
\end{aligned}
$$

and the same representations for supercores with $\mathbf{\Delta}_{ND}^{(d_k)}$ instead of $\mathbf{\Delta}_{DN}^{(d_k)}$, I_2 being replaced with I_1.

Proof.

$$\begin{bmatrix} a_k \mathbf{\Delta}_{DN}^{(d_k)} \\ I^{\otimes d_k} \end{bmatrix} = \begin{bmatrix} I & J' & J & I_2 & \\ & & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & I_2 & \\ & & & & I \end{bmatrix}^{\bowtie (d-2)} \bowtie \begin{bmatrix} a_k\left(2I - J - J'\right) \\ -a_k J \\ -a_k J' \\ -a_k I_2 \\ I \end{bmatrix}$$

$$= \begin{bmatrix} I & J' & J & I_2 & \\ & & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & I_2 & \\ & & & & I \end{bmatrix}^{\bowtie (d-3)}$$

$$\bowtie \begin{bmatrix} a_k I & a_k J' & a_k J & \\ & a_k J & & \\ & & a_k J' & \\ & & & a_k I_2 \\ \frac{1}{2} I & -\frac{1}{2} I & -\frac{1}{2} I & \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_2 \end{bmatrix},$$

proof for other supercores is similar to that of Corollary 2.4. □

Corollary 2.6. *For any $d \geq 4$ the following QTT representations hold:*

$$\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_{NN}^{(d_k)} \\ & I^{\otimes d_k} \end{bmatrix} = \begin{bmatrix} I & J' & J & I_2 & \\ & & & & I \end{bmatrix}$$

$$\bowtie \begin{bmatrix} I & J' & J & & I_1 & \\ & J & & & & \\ & & J' & & & \\ & & & I_2 & -I_1 & \\ & & & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & & \\ & J & & & & \\ & & J' & & & \\ & & & I_2 & & \\ & & & & I_1 & \\ & & & & & I \end{bmatrix}^{\bowtie (d-4)}$$

$$\bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & a_k I_2 & \\ & & & & a_k I_1 \\ & & & -I & -I \end{bmatrix} \bowtie \begin{bmatrix} I & a_k\left(2I - J - J'\right) \\ & -a_k J \\ & -a_k J' \\ & -I_2 \\ & -I_1 \end{bmatrix},$$

$$\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_{NN}^{(d_k)} \end{bmatrix} = \begin{bmatrix} I & J' & J & I_2 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & I_1 \\ & J & & & \\ & & J' & & \\ & & & I_2 & -I_1 \end{bmatrix}$$

$$\bowtie \begin{bmatrix} I & J' & J & & \\ & J & & & \\ & & J' & & \\ & & & I_2 & \\ & & & & I_1 \end{bmatrix}^{\bowtie (d-3)} \bowtie \begin{bmatrix} I & a_k\left(2I - J - J'\right) \\ & -a_k J \\ & -a_k J' \\ & -a_k I_2 \\ & -a_k I_1 \end{bmatrix},$$

$$\begin{bmatrix} a_k \mathbf{\Delta}_{NN}^{(d_k)} \\ I^{\otimes d_k} \end{bmatrix} = \begin{bmatrix} I & J' & J & I_2 & \\ & & & & I \end{bmatrix}$$

$$
\bowtie \begin{bmatrix} I & J' & J & & I_1 & \\ & J & & & & \\ & & J' & & & \\ & & & I_2 & -I_1 & \\ & & & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & & & \\ & J & & & & \\ & & J' & & & \\ & & & I_2 & & \\ & & & & I_1 & \\ & & & & & I \end{bmatrix}^{\bowtie (d-4)}
$$

$$
\bowtie \begin{bmatrix} a_k I & a_k J' & a_k J & \\ & a_k J & & \\ & & a_k J' & \\ & & & a_k I_2 \\ \frac{1}{2} a_k I_1 & -\frac{1}{2} a_k I_1 & -\frac{1}{2} a_k I_1 & -a_k I_1 \\ \frac{1}{2} I & -\frac{1}{2} I & -\frac{1}{2} I & \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_2 \end{bmatrix}.
$$

Proof. Is similar to that of Corollary 2.4 and Corollary 2.5. □

Corollary 2.7. *For any $d \geq 4$ the following QTT representations hold:*

$$
\begin{aligned}
\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_P^{(d_k)} \\ & I^{\otimes d_k} \end{bmatrix} &= \begin{bmatrix} I & P \\ & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & J' & \\ & & & I \end{bmatrix} \\
&\bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I \end{bmatrix}^{\bowtie (d-3)} \bowtie \begin{bmatrix} I & a_k \left(2I - J - J'\right) \\ & -a_k J \\ & -a_k J' \\ & I \end{bmatrix}, \\
\begin{bmatrix} I^{\otimes d_k} & a_k \mathbf{\Delta}_P^{(d_k)} \end{bmatrix} &= \begin{bmatrix} I & P \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & J' \end{bmatrix} \\
&\bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie (d-3)} \bowtie \begin{bmatrix} I & a_k \left(2I - J - J'\right) \\ & -a_k J \\ & -a_k J' \end{bmatrix}, \\
\begin{bmatrix} a_k \mathbf{\Delta}_P^{(d_k)} \\ I^{\otimes d_k} \end{bmatrix} &= \begin{bmatrix} I & P \\ & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & J' & \\ & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I \end{bmatrix}^{\bowtie (d-4)} \\
&\bowtie \begin{bmatrix} a_k I & a_k J' & a_k J \\ & a_k J & \\ & & a_k J' \\ \frac{1}{2} I & -\frac{1}{2} I & -\frac{1}{2} I \end{bmatrix} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \end{bmatrix}.
\end{aligned}
$$

Proof. Is similar to those of Corollary 2.4, Corollary 2.5 and Corollary 2.6. □

3 Inverse Laplace operator in one dimension

Next we derive low-rank QTT decompositions of inverse of a discretized Laplace operator, Dirichlet-Neumann or Dirichlet-Dirichlet boundary conditions being imposed. We will proceed from explicit representation of ${\mathbf{\Delta}_{DD}^{(d)}}^{-1}$ and ${\mathbf{\Delta}_{DN}^{(d)}}^{-1}$.

Proposition 3.1. *Let*

$$\Delta_{DD} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix}, \quad \Delta_{DN} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}$$

be $n \times n$-matrices. Then

$$\begin{aligned} {\Delta_{DD}}^{-1}{}_{ij} &= \frac{1}{n+1} \begin{cases} i(n+1-j), & 1 \le i \le j \le n \\ (n+1-i)j, & 1 \le j < i \le n \end{cases}, \\ {\Delta_{DN}}^{-1}{}_{ij} &= \frac{1}{n+1} \begin{cases} i(n+1), & 1 \le i \le j \le n \\ (n+1)j, & 1 \le j < i \le n \end{cases}. \end{aligned}$$

Proof. Follows at once from either explicit expressions of Green's functions of the corresponding Sturm-Liouville problems (see, for example, [27]) or a direct check. □

Lemma 3.2. *For any $d \ge 2$ it holds that*

$$\boldsymbol{\Delta}_{DN}^{(d)\ -1} = \begin{bmatrix} I & I_2 & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & I_2 & J & J' \\ & 2E & & \\ & I_2 + J' & E & \\ & I_2 + J & & E \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} E + I_2 \\ 2E \\ E + I_2 + J' \\ E + I_2 + J \end{bmatrix}.$$

Proof. According to Proposition 3.1, the inverse of the matrix $\boldsymbol{\Delta}_{DN}^{(d)}$ has the following form:

$$\boldsymbol{\Delta}_{DN}^{(d)\ -1} = \begin{pmatrix} 1 & \cdots & \cdots & \cdots & 1 \\ \vdots & 2 & \cdots & \cdots & 2 \\ \vdots & \vdots & 3 & \cdots & 3 \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & 2 & 3 & \cdots & 2^d \end{pmatrix}, \tag{16}$$

and hence, introducing matrices

$$\boldsymbol{K}^{(k)} = \begin{pmatrix} 1 & 2 & 3 & \cdots & 2^k \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ 1 & 2 & 3 & \cdots & 2^k \end{pmatrix},$$

$1 \le k \le D-1$, which it holds for that

$$\boldsymbol{K}^{(k)} = \left(\begin{array}{c|c} \boldsymbol{K}^{(k-1)} & 2^{k-1}E^{\otimes(k-1)} + \boldsymbol{K}^{(k-1)} \\ \hline \boldsymbol{K}^{(k-1)} & 2^{k-1}E^{\otimes(k-1)} + \boldsymbol{K}^{(k-1)} \end{array}\right) = \begin{bmatrix} I_2 + J & E \end{bmatrix} \bowtie \begin{bmatrix} 2^{k-1}E^{\otimes(k-1)} \\ \boldsymbol{K}^{(k-1)} \end{bmatrix},$$

we draw up the following:

$$
\begin{aligned}
{\mathbf{\Delta}_{DN}^{(d)}}^{-1} &= \begin{bmatrix} I & I_2 & J & J' \end{bmatrix} \bowtie \begin{bmatrix} {\mathbf{\Delta}_{DN}^{(d-1)}}^{-1} \\ 2^{d-1} E^{\otimes(d-1)} \\ \boldsymbol{K}^{(d-1)'} \\ \boldsymbol{K}^{(d-1)} \end{bmatrix} \\
&= \begin{bmatrix} I & I_2 & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & I_2 & J & J' & & & & & & & & & & & & \\ & & & & 2E & & & & & & & & & & & \\ & & & & & & & & I_2 + J' & E & & & & & & \\ & & & & & & & & & & & & I_2 + J & E & & \end{bmatrix} \\
&\bowtie \begin{bmatrix} {\mathbf{\Delta}_{DN}^{(d-2)}}^{-1} \\ 2^{d-2} E^{\otimes(d-2)} \\ \boldsymbol{K}^{(d-2)'} \\ \boldsymbol{K}^{(d-2)} \\ 2^{d-2} E^{\otimes(d-2)} \\ 2^{d-2} E^{\otimes(d-2)} \\ \boldsymbol{K}^{(d-2)'} \\ 2^{d-2} E^{\otimes(d-2)} \\ \boldsymbol{K}^{(d-2)} \end{bmatrix} = \begin{bmatrix} I & I_2 & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & I_2 & J & J' \\ & 2E & & \\ & I_2 + J' & E & \\ & I_2 + J & & E \end{bmatrix} \bowtie \begin{bmatrix} {\mathbf{\Delta}_{DN}^{(d-2)}}^{-1} \\ 2^{d-2} E^{\otimes(d-2)} \\ \boldsymbol{K}^{(d-2)'} \\ \boldsymbol{K}^{(d-2)} \end{bmatrix} \\
&= \ldots = \begin{bmatrix} I & I_2 & J & J' \end{bmatrix} \bowtie \begin{bmatrix} I & I_2 & J & J' \\ & 2E & & \\ & I_2 + J' & E & \\ & I_2 + J & & E \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} E + I_2 \\ 2E \\ E + I_2 + J' \\ E + I_2 + J \end{bmatrix}.
\end{aligned}
$$

□

Lemma 3.3. *Let $d \geq 2$ and*

$$\xi_k = \frac{2^{k-1}+1}{2^k+1}, \quad \eta_k = \frac{2^{k-2}}{2^k+1}, \quad \zeta_k = \frac{2^{k-1}+1}{2^{k-1}} \xi_k$$

for $1 \leq k \leq d$. Then ${\mathbf{\Delta}_{DD}^{(d)}}^{-1}$ has a rank-$5 \ldots 5$ QTT representation

$$ {\mathbf{\Delta}_{DD}^{(d)}}^{-1} = W_d \bowtie W_{d-1} \bowtie \ldots \bowtie W_2 \bowtie W_1, $$

which consists of the TT cores

$$
\begin{aligned}
W_d &= \begin{bmatrix} I & \frac{1}{4}\xi_d I + \frac{1}{4}\zeta_d P & \xi_d I - \zeta_d P & -\xi_d K & \zeta_d L \end{bmatrix} \\
W_k &= \begin{bmatrix} I & \frac{1}{4}\xi_k I + \frac{1}{4}\zeta_k P & \xi_k I - \zeta_k P & -\xi_k K & \zeta_k L \\ & 2E & & & \\ & 2\eta_k^2 F & 2\xi_k^2 E & 2\xi_k \eta_k K & \xi_k \eta_k L \\ & 4\eta_k K & & 2\xi_k E & \\ & -4\eta_k L & & & 2\xi_k E \end{bmatrix}, \quad 2 \leq k \leq d-1, \\
W_1 &= \begin{bmatrix} \frac{1}{3}(I+E) \\ 2E \\ \frac{1}{18}F \\ \frac{2}{3}K \\ -\frac{2}{3}L \end{bmatrix}.
\end{aligned}
$$

Proof. Let $Q^{(k)}$ be a $2^k \times 2$-matrix comprising columns 2^{k-1} and $2^{k-1}+1$ of $I^{\otimes k}$ and $D^{(k)} = I \otimes \mathbf{\Delta}_{DD}^{(k-1)}$. Then, as it is plain to see from (4),

$$\mathbf{\Delta}_{DD}^{(k)} = I \otimes \mathbf{\Delta}_{DD}^{(k-1)} - Q^{(k)} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} Q^{(k)\prime},$$

and, according to the Sherman-Morrison-Woodbury formula [6, p. 51],

$$\begin{aligned} \mathbf{\Delta}_{DD}^{(k)\,-1} &= I \otimes \mathbf{\Delta}_{DD}^{(k-1)^{-1}} + A^{(k)}, \qquad (17) \\ A^{(k)} &= D^{(k)^{-1}} Q^{(k)} B^{(k)} Q^{(k)\prime} D^{(k)^{-1}}, \\ B^{(k)} &= \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^{-1} - Q^{(k)\prime} D^{(k)^{-1}} Q^{(k)} \right)^{-1}, \end{aligned}$$

where $D^{(k)^{-1}} = I \otimes \mathbf{\Delta}_{DD}^{(k-1)^{-1}}$, and using Proposition 3.1 we arrive at

$$\begin{aligned} B^{(k)} &= \begin{pmatrix} -\frac{2^{k-1}}{2^{k-1}+1} & 1 \\ 1 & -\frac{2^{k-1}}{2^{k-1}+1} \end{pmatrix}^{-1} = \frac{2^{k-1}+1}{2^k+1} \begin{pmatrix} 2^{k-1} & 2^{k-1}+1 \\ 2^{k-1}+1 & 2^{k-1} \end{pmatrix} = 2^{k-1} \begin{pmatrix} \xi_k & \zeta_k \\ \zeta_k & \xi_k \end{pmatrix} \\ &= 2^{k-1} \left(\xi_k I + \zeta_k P \right). \end{aligned}$$

Next, we define 2^k-component vectors

$$e^{(k)} = 2^k \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \quad \text{and} \quad z^{(k)} = \frac{2^k}{2^k+1} \begin{pmatrix} 1 \\ \vdots \\ 2^k \end{pmatrix} - \frac{1}{2} e^{(k)} = \frac{1}{2} \cdot \frac{2^k}{2^k+1} \begin{pmatrix} 1-2^k \\ \vdots \\ 2^k-1 \end{pmatrix},$$

$x^{(k)} = \frac{1}{2} e^{(k)} + z^{(k)}$ and $y^{(k)} = \frac{1}{2} e^{(k)} - z^{(k)}$. Then, according to Proposition 3.1, $2^{-k} x^{(k)}$ and $2^{-k} y^{(k)}$ are respectively the last and the first columns of $\mathbf{\Delta}_{DD}^{(k)\,-1}$; $2^{-k} x^{(k)\prime}$ and $2^{-k} y^{(k)\prime}$, rows, $k \geq 2$, and hence

$$A^{(k)} = \frac{1}{2^{k-1}} \left(\begin{array}{c|c} x^{(k-1)} x^{(k-1)\prime} & \zeta_k x^{(k-1)} y^{(k-1)\prime} \\ \hline \zeta_k y^{(k-1)} x^{(k-1)\prime} & y^{(k-1)} y^{(k-1)\prime} \end{array} \right). \qquad (18)$$

Now let us express the blocks involved in the last equality in terms of the vectors $e^{(k-1)}$ and $z^{(k-1)}$. For any $k \geq 2$ it holds by definition of $x^{(k)}$ and $y^{(k)}$ that

$$\begin{aligned} x^{(k)} x^{(k)\prime} &= \frac{1}{4} e^{(k)} e^{(k)\prime} + \frac{1}{2} \left(e^{(k)} z^{(k)\prime} + z^{(k)} e^{(k)\prime} \right) + z^{(k)} z^{(k)\prime}, \\ y^{(k)} y^{(k)\prime} &= \frac{1}{4} e^{(k)} e^{(k)\prime} - \frac{1}{2} \left(e^{(k)} z^{(k)\prime} + z^{(k)} e^{(k)\prime} \right) + z^{(k)} z^{(k)\prime}, \\ x^{(k)} y^{(k)\prime} &= \frac{1}{4} e^{(k)} e^{(k)\prime} - \frac{1}{2} \left(e^{(k)} z^{(k)\prime} - z^{(k)} e^{(k)\prime} \right) - z^{(k)} z^{(k)\prime}, \\ y^{(k)} x^{(k)\prime} &= \frac{1}{4} e^{(k)} e^{(k)\prime} + \frac{1}{2} \left(e^{(k)} z^{(k)\prime} - z^{(k)} e^{(k)\prime} \right) - z^{(k)} z^{(k)\prime}. \qquad (19) \end{aligned}$$

The right-hand matrices have simple recursive structure. Indeed,

$$e^{(k)} = 2 \left(\frac{e^{(k-1)}}{e^{(k-1)}} \right) \quad \text{and} \quad z^{(k)} = 2 \left(\frac{\xi_k z^{(k-1)} - \eta_k e^{(k-1)}}{\xi_k z^{(k-1)} + \eta_k e^{(k-1)}} \right),$$

therefore

$$e^{(k)} e^{(k)\prime} = 4E \otimes e^{(k-1)} e^{(k-1)\prime},$$

$$\begin{aligned}
z^{(k)}z^{(k)\prime} &= 4\xi_k^2 E\otimes z^{(k-1)}z^{(k-1)\prime} + 4\eta_k^2 F\otimes e^{(k-1)}e^{(k-1)\prime} \\
&+ 4\xi_k\eta_k K\otimes\left(e^{(k-1)}z^{(k-1)\prime} + z^{(k-1)}e^{(k-1)\prime}\right) \\
&+ 4\xi_k\eta_k L\otimes\left(e^{(k-1)}z^{(k-1)\prime} - z^{(k-1)}e^{(k-1)\prime}\right) \\
e^{(k)}z^{(k)\prime} + z^{(k)}e^{(k)\prime} &= 8\eta_k K\otimes e^{(k-1)}e^{(k-1)\prime} \\
&+ 4\xi_k E\otimes\left(e^{(k-1)}z^{(k-1)\prime} + z^{(k-1)}e^{(k-1)\prime}\right) \\
e^{(k)}z^{(k)\prime} - z^{(k)}e^{(k)\prime} &= -8\eta_k L\otimes e^{(k-1)}e^{(k-1)\prime} \\
&+ 4\xi_k E\otimes\left(e^{(k-1)}z^{(k-1)\prime} - z^{(k-1)}e^{(k-1)\prime}\right),
\end{aligned}$$

and in core notation this can be recast to

$$\frac{1}{2^k}\begin{bmatrix} e^{(k)}e^{(k)\prime} \\ z^{(k)}z^{(k)\prime} \\ e^{(k)}z^{(k)\prime} + z^{(k)}e^{(k)\prime} \\ e^{(k)}z^{(k)\prime} - z^{(k)}e^{(k)\prime} \end{bmatrix} = V_k \bowtie \frac{1}{2^{k-1}}\begin{bmatrix} e^{(k-1)}e^{(k-1)\prime} \\ z^{(k-1)}z^{(k-1)\prime} \\ e^{(k-1)}z^{(k-1)\prime} + z^{(k-1)}e^{(k-1)\prime} \\ e^{(k-1)}z^{(k-1)\prime} - z^{(k-1)}e^{(k-1)\prime} \end{bmatrix}$$

with the cores V_k, $k \geq 2$, defined as

$$V_k = \begin{bmatrix} 2E & & & \\ 2\eta_k^2 F & 2\xi_k^2 E & 2\xi_k\eta_k K & 2\xi_k\eta_k L \\ 4\eta_k K & & 2\xi_k E & \\ -4\eta_k L & & & 2\xi_k E \end{bmatrix}$$

As long as this holds for any $k \geq 2$ and $e^{(1)}e^{(1)\prime} = 4E$, $z^{(1)}z^{(1)\prime} = \frac{1}{9}F$, $e^{(1)}z^{(1)\prime} + z^{(1)}e^{(1)\prime} = \frac{4}{3}K$, $e^{(1)}z^{(1)\prime} - z^{(1)}e^{(1)\prime} = -\frac{4}{3}L$, we conclude that

$$\frac{1}{2^k}\begin{bmatrix} e^{(k)}e^{(k)\prime} \\ z^{(k)}z^{(k)\prime} \\ e^{(k)}z^{(k)\prime} + z^{(k)}e^{(k)\prime} \\ e^{(k)}z^{(k)\prime} - z^{(k)}e^{(k)\prime} \end{bmatrix} = V_k \bowtie \ldots \bowtie V_2 \bowtie V_1, \quad V_1 = \begin{bmatrix} 2E \\ \frac{1}{18}F \\ \frac{2}{3}K \\ -\frac{2}{3}L \end{bmatrix}. \tag{20}$$

Now we introduce

$$\Gamma_k = \begin{bmatrix} \frac{1}{4}\xi_k I + \frac{1}{4}\zeta_k P & \xi_k I - \zeta_k P & -\xi_k K & \zeta_k L \end{bmatrix},$$

$k \geq 2$, and join (18), (19) and (20):

$$\begin{aligned}
A^{(k)} &= \Gamma_k \bowtie \frac{1}{2^{k-1}}\begin{bmatrix} e^{(k-1)}e^{(k-1)\prime} \\ z^{(k-1)}z^{(k-1)\prime} \\ e^{(k-1)}z^{(k-1)\prime} + z^{(k-1)}e^{(k-1)\prime} \\ e^{(k-1)}z^{(k-1)\prime} - z^{(k-1)}e^{(k-1)\prime} \end{bmatrix} \\
&= \Gamma_k \bowtie V_{k-1} \bowtie \ldots \bowtie V_1
\end{aligned}$$

Applying (17) recursively, we attain the following expression for ${\mathbf{\Delta}_{DD}^{(d)}}^{-1}$:

$${\mathbf{\Delta}_{DD}^{(d)}}^{-1} = I^{\otimes(d-1)} \otimes {\mathbf{\Delta}_{DD}^{(1)}}^{-1} + \sum_{k=2}^{d} I^{\otimes(d-k)} \otimes A^{(k)}.$$

Let $U_k = \left[I \right]$, $1 \le k \le d$, $\Gamma_1 = \left[{\mathbf{\Delta}_{DD}^{(1)}}^{-1} \right]$, then

$$\begin{aligned}
{\mathbf{\Delta}_{DD}^{(d)}}^{-1} &= U_d \bowtie U_{d-1} \bowtie U_{d-2} \bowtie \ldots \bowtie U_3 \bowtie U_2 \bowtie \Gamma_1 \\
&+ U_d \bowtie U_{d-1} \bowtie U_{d-2} \bowtie \ldots \bowtie U_3 \bowtie \Gamma_2 \bowtie V_1 \\
&+ \ldots \\
&+ U_d \bowtie \Gamma_{d-1} \bowtie V_{d-2} \bowtie \ldots \bowtie V_3 \bowtie V_2 \bowtie V_1 \\
&+ \Gamma_d \bowtie V_{d-1} \bowtie V_{d-2} \bowtie \ldots \bowtie V_3 \bowtie V_2 \bowtie V_1,
\end{aligned}$$

which can be represented as following in accordance with Lemma 1.3:

$$ {\mathbf{\Delta}_{DD}^{(d)}}^{-1} = \left[I \;\middle|\; \Gamma_d \right] \bowtie \left[\begin{array}{c|c} I & \Gamma_{d-1} \\ \hline & V_{d-1} \end{array} \right] \bowtie \ldots \bowtie \left[\begin{array}{c|c} I & \Gamma_2 \\ \hline & V_2 \end{array} \right] \bowtie \left[\begin{array}{c} \Gamma_1 \\ \hline V_1 \end{array} \right]. $$

That is the QTT representation was to be proven. □

It is obvious that the rank-$5 \ldots 5$ representation given by Lemma 3.3 is a little excessive since it has ranks of terminal cores are greater than 4, which is trivial to amend. Let us now get rid of this redundancy and obtain a rank-$4, 5 \ldots 5, 4$ decomposition.

Remark 3.4. Lemma 3.3 holds for $d \ge 4$, the cores W_d, W_{d-1}, W_2, W_1 being the following:

$$\begin{aligned}
W_d &= \begin{bmatrix} \frac{1}{4}\xi_d I + \frac{1}{4}\zeta_d P & \xi_d I - \zeta_d P & -\xi_d K & \zeta_d L \end{bmatrix} \\
W_{d-1} &= \begin{bmatrix} \frac{2}{\xi_d} & 1 & & & \\ \frac{1}{2\xi_d} & & 1 & & \\ & & & 1 & \\ & & & & 1 \end{bmatrix} \\
&\bowtie \begin{bmatrix} I & \frac{1}{4}\xi_{d-1} I + \frac{1}{4}\zeta_{d-1} P & \xi_{d-1} I - \zeta_{d-1} P & -\xi_{d-1} K & \zeta_{d-1} L \\ & 2E & & & \\ & 2\eta_{d-1}^2 F & 2\xi_{d-1}^2 E & 2\xi_{d-1}\eta_{d-1} K & \xi_{d-1}\eta_{d-1} L \\ & 4\eta_{d-1} K & & 2\xi_{d-1} E & \\ & -4\eta_{d-1} L & & & 2\xi_{d-1} E \end{bmatrix}, \\
W_2 &= \begin{bmatrix} \frac{1}{4}\xi_2 I + \frac{1}{4}\zeta_2 P + \frac{1}{4} I & \xi_2 I - \zeta_2 P + 3I & -\xi_2 K & \zeta_2 L \\ 2E & & & \\ 2\eta_2^2 F & 2\xi_2^2 E & 2\xi_2\eta_2 K & \xi_2\eta_2 L \\ 4\eta_2 K & & 2\xi_2 E & \\ -4\eta_2 L & & & 2\xi_2 E \end{bmatrix}, \\
W_1 &= \begin{bmatrix} 2E \\ \frac{1}{18} F \\ \frac{2}{3} K \\ -\frac{2}{3} L \end{bmatrix}.
\end{aligned}$$

4 Vector QTT rank estimates

Let us now recur to the equations (1) and (2) and set forth some QTT ranks estimates appearing from our results obtained in the previous sections.

Theorem 4.1. *The following upper bounds of vector QTT ranks of the corresponding matrices hold.*

$$
\begin{array}{rcl}
\mathbf{\Delta}_{DD}^{(d)} & : & 3 \dots 3 \\
 & & \textit{(Lemma 2.1)} \\
\mathbf{\Delta}_{DN}^{(d)},\ \mathbf{\Delta}_{ND}^{(d)} & : & 4 \dots 4 \\
\mathbf{\Delta}_{NN}^{(d)} & : & 4, 5 \dots 5, 4 \\
\mathbf{\Delta}_{P}^{(d)} & : & 2, 3 \dots 3 \\
 & & \textit{(Lemma 2.2)} \\
{\mathbf{\Delta}_{DD}^{(d)}}^{-1} & : & 4, 5 \dots 5, 4 \\
 & & \textit{(Lemma 3.3 and Remark 3.4)} \\
{\mathbf{\Delta}_{DN}^{(d)}}^{-1},\ {\mathbf{\Delta}_{ND}^{(d)}}^{-1} & : & 4 \dots 4 \\
 & & \textit{(Lemma 3.2)} \\
\mathbf{\Delta}_{DD}^{(d_1 \dots d_d)} & : & 3 \dots 3, \mathbf{2}, 4 \dots 4, \mathbf{2} \dots \dots \mathbf{2}, 4 \dots 4, \mathbf{2}, 4 \dots 4, 3 \\
 & & \textit{(Corollary 2.4)} \\
\mathbf{\Delta}_{DN}^{(d_1 \dots d_d)},\ \mathbf{\Delta}_{ND}^{(d_1 \dots d_d)} & : & 4 \dots 4, \mathbf{2}, 5 \dots 5, \mathbf{2} \dots \dots \mathbf{2}, 5 \dots 5, \mathbf{2}, 5 \dots 5, 4 \\
 & & \textit{(Corollary 2.5)} \\
\mathbf{\Delta}_{NN}^{(d_1 \dots d_d)} & : & 4, 5 \dots 5, \mathbf{2}, 5, 6 \dots 6, 5, \mathbf{2} \dots \dots \mathbf{2}, 5, 6 \dots 6, 5, \mathbf{2}, 5, 6 \dots 6, 4 \\
 & & \textit{(Corollary 2.6)} \\
\mathbf{\Delta}_{P}^{(d_1 \dots d_d)} & : & 2, 3 \dots 3, \mathbf{2}, 3, 4 \dots 4, \mathbf{2} \dots \dots \mathbf{2}, 3, 4 \dots 4, \mathbf{2}, 3, 4 \dots 4, 3 \\
 & & \textit{(Corollary 2.7)}
\end{array}
$$

Proof. Follows straighforwardly from the lemmas, corollaries and the remark referred and presenting explicit QTT representation of the mentioned ranks. □

Remark 4.2. Numerical experiments carried out with Ivan Oseledets'[1] TT Toolbox[2] prove all the upper bounds for vector QTT ranks given in Theorem 4.1 to be sharp; the corresponding explicit representations, to be of minimal rank.

5 Operator TT rank

In Introduction we considered vector TT rank of matrices in view of storage costs and complexity of the basic operations. But, on the other hand, even if we manage to perform, for instance, a matrix-by-vector multiplication, this may not be enough for solution of the problem involved. For example, developing iterative solvers we are likely to be concerned with vector TT ranks of a matrix-by-vector product, which is certainly the case in Krylov subspace methods. Formally, ranks of TT decompositions are multiplied when two matrices or a matrix and a vector are multiplied. But often this obvious estimate of ranks of the product leads to unaffordable complexity estimates, but, fortunately, is not sharp, so that low-rank approximation is possible with an endurable error [4]. A reasonable a priori estimate of ranks would allow one to rely upon such the approximation procedure,

[1] Institute of Numerical Mathematics, Russian Academy of Sciences. Moscow, Russia

[2] Available for free at `http://spring.inm.ras.ru/osel`

complexity of which is cubic in respect of ranks. That is why we are also to take into account *operator TT rank* defined below.

Definition 5.1. A multi-way matrix $\boldsymbol{A} : \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_D} \mapsto \mathbb{R}^{m_1} \times \ldots \times \mathbb{R}^{m_D}$ given, for any vector $\boldsymbol{X} \in \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_D}$ let us denote vector TT ranks of the matrix-by-vector product $\boldsymbol{AX}$ by $r_1 \ldots r_{D-1}$. Then let us refer to

$$\max_{\substack{k=1\ldots D-1,\\ \boldsymbol{X} \text{ is of vector TT rank } 1\ldots 1}} r_k$$

as the *operator TT rank* of $\boldsymbol{A}$.

Actually we have already arrived above at the following obvious inequality between the two ranks introduced in Definition 0.2 and Definition 5.1.

Proposition 5.2. *Operator TT rank does not exceed the maximum component of vector TT rank.*

This estimate is essentially not sharp. For example, consider two vectors $\boldsymbol{X}, \boldsymbol{Y} \in \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_D}$ such that $\boldsymbol{X}$ is of vector TT rank $1 \ldots 1$. Then for any vector $\boldsymbol{Z} \in \mathbb{R}^{n_1} \times \ldots \times \mathbb{R}^{n_D}$ of vector TT rank $1 \ldots 1$ the tensor $(\boldsymbol{XY}')\,\boldsymbol{Z} = \langle \boldsymbol{Y}, \boldsymbol{Z} \rangle\, \boldsymbol{X}$ is of vector TT rank $1 \ldots 1$, while $(\boldsymbol{YX}')\,\boldsymbol{Z} = \langle \boldsymbol{X}, \boldsymbol{Z} \rangle\, \boldsymbol{Y}$ is of the same vector TT rank as $\boldsymbol{Y}$. Consequently, operator TT rank of $\boldsymbol{XY}'$ is equal to 1, while that of $\boldsymbol{YX}'$ is as high as the maximum rank of TT cores of $\boldsymbol{Y}$, which can be random and have a very bad QTT structure resulting in a high vector TT rank of $\boldsymbol{XY}'$.

6 Relation to multigrid

The representations obtained above highlight a close relation between Quantics Tensor Train and multigrid methods. For example, in order to proceed to a twice finer grid one need just to put another core in the middle of the tensor train involved in the decompositions given by Lemma 2.1, Lemma 2.2, Lemma 3.2, and this extra core is exactly the same as the ones present in the initial tensor train. For the decomposition of $\boldsymbol{\Delta}^{(d)}_{DD}$ given by Lemma 3.3 this is slightly more complicated, but still very similar. This observation leads to the idea of using QTT along with multigrid techniques in high-dimensional problems on fine grids. But this idea involves also restriction and prolongation of vectors, and QTT structure of the corresponding operators is of interest too.

Example 6.1. *Consider a one-dimensional problem over* $[0, 1]$ *with a Dirichlet boundary condition at* 0 *and non-Dirichlet one at* 1*, discretized on a sequence of grids* $x^{(k)}$*:* $x^{(k)}_i = \frac{i}{2^k}$, $1 \leq i \leq 2^k$*, by means of Finite Element Method with base functions*

$$x \mapsto \varphi^{(k)}_i(x) = \begin{cases} 1 + \frac{1}{2^k}\left(x - x^{(k)}_i\right), & x \in \left(x^{(k)}_{i-1}, x^{(k)}_i\right] \cap [0,1], \\ 1 - \frac{1}{2^k}\left(x - x^{(k)}_i\right), & x \in \left(x^{(k)}_i, x^{(k)}_{i+1}\right] \cap [0,1], \\ 0, & \textit{otherwise}. \end{cases}$$

Let us define a prolongation operator from $\operatorname{span}\left\{\varphi_i^{(d)}\right\}_{i=1}^{2^d}$ *to* $\operatorname{span}\left\{\varphi_i^{(d-1)}\right\}_{i=1}^{2^{d-1}}$ *so that its* $2^d \times 2^{d-1}$*-matrix is*

$$\boldsymbol{P}^{(d)} = \begin{pmatrix} \frac{1}{2} & & & \\ 1 & & & \\ \frac{1}{2} & \frac{1}{2} & & \\ & 1 & & \\ & \frac{1}{2} & \ddots & \\ & & \ddots & \frac{1}{2} \\ & & \ddots & 1 \\ & & & \frac{1}{2} & \frac{1}{2} \\ & & & & 1 \end{pmatrix}$$

and a restriction operator with a matrix $\boldsymbol{R}^{(d)} = \frac{1}{2}\boldsymbol{P}^{(d)\prime}$. *Then it is easy to draw up a rank-*$2\ldots2$ *QTT-like decomposition of* $\boldsymbol{P}^{(d)}$ *similarly to as we did it with QTT decompositions of shift and gradient matrices in the section 1.2:*

$$\boldsymbol{P}^{(d)} = \begin{bmatrix} I & J' \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{P}^{(d-1)} \\ \frac{1}{2} J^{\otimes(d-2)} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{bmatrix} = \ldots = \frac{1}{2} \begin{bmatrix} I & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J' \\ & J \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} \\ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{bmatrix},$$

and hence

$$\boldsymbol{R}^{(d)} = \frac{1}{4} \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix}^{\bowtie(d-2)} \bowtie \begin{bmatrix} \begin{pmatrix} 1 & 2 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \end{pmatrix} \end{bmatrix}.$$

This is by far the most simple example of geometric multigrid approach considering a problem with 2^d unknowns on the d-th grid, and in a more general case prolongation and restriction operators may not have such a nice QTT-like structure.

Conclusion

We have investigated QTT ranks and explicit structure of Laplace operator for various boundary conditions in D dimensions, taking into account the anisotropy involved in (3). Though representations and rank estimates can be obtained numerically, our results allow one to avoid these computations which can be rather expensive and not precise enough, D and, especially, d being very high. “One-dimensional” inverse Laplace operators for Dirichlet and Dirichlet-Neumann boundary condition has been also considered and represented in the QTT format with a low rank and well-balanced TT cores.

We believe that this work contributes to comprehension of the Tensor Train format and its “tensorized” version, the Quantics Tensor Train format, as long as it is the first paper on explicit QTT representation of operators, and we hope that further research would allow one to put forward new ideas of solving particular problems of scientific computing.

On the other hand, while deriving the explicit QTT representations presented in the paper and performing numerical experiments with them we found out that QTT fits some special matrices quite well. Experiments prove inverse of a tridiagonal Toeplitz matrix to have vector QTT rank $4, 5 \ldots 5, 4$, and it seems that Lemma 3.3 can be generalized to this case. This result for discretized Laplace operator and observations for Toeplitz matrices conform to the theorem stated in [28] and asserting that inverse of a band Toeplitz matrix of bandwidth s has vector QTT ranks bounded above by $4s^2 + 1$. In a way, this topic marries applications of QTT in scientific computing and the algebraic point of view on it and hence is of great interest for further research.

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