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LOW-RANK EXPLICIT QTT REPRESENTATION OF THE LAPLACE OPERATOR AND ITS INVERSE*

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Abstract. We focus on the construction of explicit low-rank representations of matrices in the tensor train (TT) and quantized tensor train (QTT) formats which have been proposed recently for the low-parametric structured representation of large-scale tensors. The matrices under consideration are discretizations of the Laplace operator in a hypercube (in one and many dimensions) and their inverses (in one dimension). For these matrices we derive explicit and exact QTT representations of low QTT ranks independent of the numbers d and n^2 of dimensions and entries in each dimension. This implies that for the matrices considered the storage cost is $\mathcal{O}\left(d \log n\right)$, i.e., logarithmic with respect to the total number n^{2d} of entries. The same applies to the computational complexity of the QTT-structured operations with these matrices, which now depends on the QTT ranks of the other operands. The general result of the paper is the notation and technique we introduce in order to examine the QTT structure of matrices analytically. They prove to be an efficient tool of studying other tensors related to particular computational problems, which are not considered in this paper.

Key words. tensor decompositions, tensor rank, low-rank representation, tensor train (TT), quantized tensor train (QTT), virtual levels, discrete Laplace operator

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1. Introduction. Nonlinear low-parametric approximations of multidimensional arrays, or *tensors*, find numerous applications in data analysis [26, 5, 1] and scientific computing [20]. This happens due to the complications observed in relation to high dimensions in several areas of mathematics and referred to as the "curse of dimensionality" since [3].

The key approach exploited by *tensor methods* is the reduction (exact or approximate) of tensors to their *low-rank* representations in a certain format. From a practical point of view, we are mostly interested in efficient numerical methods for obtaining such representations. However, even if they are available for a particular tensor format in use, we may prefer to represent some tensors exactly and explicitly. The obvious aim is to avoid the errors of the numerical approximation. A more important reason is that explicit low-rank representations may give rise to efficient (and explicit) algorithms in the corresponding tensor formats. This is why we are interested in the analytical construction of such tensor representations.

In this paper we are concerned with representing certain matrices in the tensor train (TT) and quantized tensor train (QTT) formats. The matrices we consider are discretizations of the negative Laplace operator in a d-dimensional hypercube with homogeneous Dirichlet or mixed Dirichlet–Neumann boundary conditions, constructed on tensor-product uniform meshes by the finite difference and finite element

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methods. For the latter method we assume that the standard "hat" functions are used in each dimension for the piecewise-linear approximation, and the multidimensional finite elements are tensor products of these functions. Consequently, the d-dimensional matrices we consider are of the form

$$\boldsymbol{\Delta}^{(l_1 \dots l_d)} = a_1\, \boldsymbol{S}_1^{(l_1)} \otimes \boldsymbol{M}_2^{(l_2)} \otimes \cdots \otimes \boldsymbol{M}_d^{(l_d)} + \cdots + \boldsymbol{M}_1^{(l_1)} \otimes \cdots \otimes \boldsymbol{M}_{d-1}^{(l_{d-1})} \otimes a_d\, \boldsymbol{S}_d^{(l_d)}, \tag{1.1}$$

where the right-hand side consists of d terms involving one-dimensional mass and stiffness matrices $\boldsymbol{M}_k^{(l_k)}$ and $\boldsymbol{S}_k^{(l_k)}$ of size $2^{l_k} \times 2^{l_k}$ for $k = 1, \dots, d$. The stiffness matrices $\boldsymbol{S}_k^{(l_k)}$, $1 \le k \le d$, are the same for both the FDM and FEM discretizations: either

$$\boldsymbol{\Delta}_{\mathrm{DD}}^{(l_k)} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{pmatrix} \quad \text{or} \quad \boldsymbol{\Delta}_{\mathrm{DN}}^{(l_k)} = \begin{pmatrix} 2 & -1 & & & \\ -1 & 2 & \ddots & & \\ & \ddots & \ddots & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{pmatrix}, \tag{1.2}$$

where "DD" and "DN" stands for the Dirichlet and Dirichlet–Neumann boundary conditions, respectively. The mass matrices $\boldsymbol{M}_k^{(l_k)}$, $1 \le k \le d$, have a similar form: $\mathbb{I}_{2^{l_k}}$ for FDM and

$$\boldsymbol{M}_{\mathrm{DD}}^{(l_k)} = \begin{pmatrix} 4 & 1 & & & \\ 1 & 4 & \ddots & & \\ & \ddots & \ddots & 1 & \\ & & 1 & 4 & 1 \\ & & & 1 & 4 \end{pmatrix} \quad \text{or} \quad \boldsymbol{M}_{\mathrm{DN}}^{(l_k)} = \begin{pmatrix} 4 & 1 & & & \\ 1 & 4 & \ddots & & \\ & \ddots & \ddots & 1 & \\ & & 1 & 4 & 1 \\ & & & 1 & 2 \end{pmatrix} \tag{1.3}$$

for FEM. In [16] we also considered the Neumann and periodic boundary conditions, but for the sake of readability these very similar cases are omitted from the present paper. Inequalities of the mesh width in different dimensions and the possible anisotropy of the Laplace operator are taken into account through the coefficients a_k, $k = 1, \dots, d$.

If the elementwise equality

$$\boldsymbol{a}_{i_1,\dots,i_d} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} U_1(i_1, \alpha_1) \cdot U_2(\alpha_1, i_2, \alpha_2) \cdot \cdots \cdot U_{d-1}(\alpha_{d-2}, i_{d-1}, \alpha_{d-1}) \cdot U_d(\alpha_{d-1}, i_d) \tag{1.4}$$

holds for a d-dimensional $n_1 \times \cdots \times n_d$-vector $\boldsymbol{a}$, it is said to be represented in the TT format in terms of *TT cores* U_k, $k = 1, \dots, d$, each of them depending on the corresponding *mode index* i_k and one or two *rank indices*. The summation limits $r_1, \dots, r_{d-1}$ are called *TT ranks* of the decomposition [33, 32]. The minimal possible ranks of a TT decomposition of a vector are referred to as *TT ranks of the vector*.

Also, one may adopt the *quantized tensor train (QTT) format* [30, 19, 31], which is the TT format applied to a vector after virtual dimensions are introduced by reshaping it to smaller mode sizes (for example, $n_k = 2$). The TT representation obtained in this way and its ranks are called a *QTT representation* of the vector and *QTT ranks* of the representation. In this sense (1.4) with $n_1 = \cdots = n_d = 2$ also implies a QTT decomposition of a one-dimensional 2^d-component vector $\overline{\boldsymbol{a}}$ with elements $\overline{\boldsymbol{a}}_i = \boldsymbol{a}_{i_1,\ldots,i_d}$, where $i = \overline{i_1 \ldots i_d} = 1 + \sum_{k=1}^{d} 2^{d-k}\,(i_k - 1)$. In the same way the QTT decomposition is applied to multidimensional vectors: for $k = 1, \ldots, d$ the kth real dimension is replaced by l_k virtual dimensions, and the resulting tensor is represented in the TT format. Both the decompositions may be also applied to a d-dimensional matrix $\boldsymbol{A}$ of size $(m_1 \times \cdots \times m_d) \times (n_1 \times \cdots \times n_d)$; for example, the TT format reads

$$\boldsymbol{A}_{\substack{i_1,\ldots,i_d\\ j_1,\ldots,j_d}} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{d-1}=1}^{r_{d-1}} U_1\,(i_1, j_1, \alpha_1) \cdot U_2\,(\alpha_1, i_2, j_2, \alpha_2) \cdot \cdots \cdot U_{d-1}\,(\alpha_{d-2}, i_{d-1}, j_{d-1}, \alpha_{d-1}) \cdot U_d\,(\alpha_{d-1}, i_d, j_d)\,, \tag{1.5}$$

where cores, ranks, and unfoldings are defined similarly to the vector case (for further details, see [31]).

To avoid confusion, below we use d and l (or l_k) to denote the numbers of real and virtual dimensions, respectively.

The concept of TT ranks is crucial in view of storage costs and complexity of all the basic operations in the TT format, such as the dot product, multidimensional contraction, matrix-vector multiplication, rank reduction, and orthogonalization of a decomposition. For the sake of simplicity, let us assume $m_k = n_k = n$ for $1 \le k \le d$; then the complexity of those operations can be estimated from above by a polynomial in the upper bound of the TT ranks of the decompositions used in computations with the factor of dn^2 [32]. If we also assume that $n = 2^l$ and that the QTT ranks are bounded with respect to d and l, then the storage cost and complexity of basic operations are $\mathcal{O}\,(d\,l)$, i.e., logarithmic with respect to n.

In this paper we construct explicit and exact QTT representations of the matrices from (1.2)–(1.3) and ${\boldsymbol{\Delta}^{(l)}_{\mathrm{DD}}}^{-1}$, ${\boldsymbol{\Delta}^{(l)}_{\mathrm{DN}}}^{-1}$ as well. For example, regarding $\boldsymbol{\Delta}^{(l)}_{\mathrm{DD}}$ this implies that we suggest QTT cores $U_1, \ldots, U_l$ such that

$$\boldsymbol{\Delta}^{(l)}_{\mathrm{DD}\,\substack{\overline{i_1,\ldots,i_l}\\ \overline{j_1,\ldots,j_l}}} = \sum_{\alpha_1=1}^{r_1} \cdots \sum_{\alpha_{l-1}=1}^{r_{l-1}} U_1\,(i_1, j_1, \alpha_1) \cdot U_2\,(\alpha_1, i_2, j_2, \alpha_2) \cdot \cdots \cdot U_{l-1}\,(\alpha_{l-2}, i_{l-1}, j_{l-1}, \alpha_{l-1}) \cdot U_l\,(\alpha_{l-1}, i_l, j_l)\,, \tag{1.6}$$

where the QTT ranks are $r_1 = \cdots = r_{l-1} = 3$. Similarly, the QTT ranks of all of the six one-dimensional matrices are shown to be bounded from above by 5 independently of l.

We also construct a TT representation of the discrete Laplace operator (1.1) in terms of the one-dimensional stiffness and mass matrices. The representation is of TT ranks $2, \ldots, 2$, which are minimal possible for every nontrivial choice of the one-dimensional matrices. Next we combine this result with the QTT representations of the one-dimensional stiffness and mass matrices to obtain QTT decompositions of the discrete d-dimensional Laplace operator. The QTT ranks of the latter are bounded by 8 for both the FDM and FEM discretizations and both the Dirichlet and mixed Dirichlet–Neumann boundary conditions.

Note that the straightforward discretizations of the Laplace operator we consider turn out to be very efficient in tensor-structured solvers based on the TT, QTT, and hierarchical tensor [15, 13] formats and yield convincing experimental results when constructed on fine meshes; see the papers [24, 8, 2, 29] on elliptic PDEs and eigenvalue problems, [7, 11] on parabolic PDEs, [21] on a nonlinear EVP, [28] on multiparametric problems, [25, 23] on stochastic PDEs, [22] on problems in quantum molecular dynamics, [18] on electronic structure calculations, and also the numerical experiments in [27, 9].

2. Notation and the explicit rank reduction. The structure that we refer to as the TT decomposition, in fact, has been known as *matrix product states (MPS)* and exploited by physicists to describe quantum spin systems for almost two decades (see [39, 36]; cf. [37]). The MPS notation suggests the interpretation of the right-hand side of (1.4) as the matrix product $U_1^{(i_1)} \cdot U_2^{(i_2)} \cdot \dots \cdot U_{d-1}^{(i_{d-1})} \cdot U_d^{(i_d)}$ of a row, $d-2$ matrices, and a column indexed by rank indices $\alpha_1, \dots, \alpha_{d-1}$ and depending also on mode indices $i_1, \dots, i_d$ as parameters. Similarly, the notation of *matrix product operators* [35] reads the right-hand side of (1.5) as a product of a row, $d-2$ matrices, and a column depending on mode indices $i_1, j_1, \dots, i_d, j_d$ as parameters. In our considerations we examine linear dependence in such matrix products considered for all possible values of the mode indices. For this reason, we introduce the following notation, which allows us to omit the mode indices correctly.

Core matrices and the rank core product. By a TT *core* of rank $p \times q$ and mode size $m \times n$ we mean a four-dimensional array with two *rank indices* varied in the ranges $1, \dots, p$ and $1, \dots, q$ and two *mode indices* varied in the ranges $1, \dots, m$ and $1, \dots, n$.

Consider a TT core U of rank $p \times q$ and mode size $m \times n$. Assume that $m \times n$-matrices $A_{\alpha\beta}$, $\alpha = 1, \dots, p$, $\beta = 1, \dots, q$, are TT *blocks* of the core U, i.e., $U(\alpha, i, j, \beta) = (A_{\alpha\beta})_{ij}$ for all values of rank indices α, β and mode indices i, j. Then the core U can be considered as the matrix

$$\begin{bmatrix} A_{11} & \cdots & A_{1q} \\ \vdots & \vdots & \vdots \\ A_{p1} & \cdots & A_{pq} \end{bmatrix}, \tag{2.1}$$

which we refer to as the *core matrix* of U. In order to avoid confusion we use parentheses for ordinary matrices, which consist of numbers and are multiplied as usual, and square brackets for cores (core matrices), which consist of blocks and are multiplied by means of the rank core product "$\bowtie$" defined below. Addition of cores is meant elementwise. Also, we may think of $A_{\alpha\beta}$ or any submatrix of the core matrix in (2.1) as *subcores* of U.

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

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

of mode size $m_1 m_2 \times n_1 n_2$.

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

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

The representation (1.5) may be recast with the use of the rank core product in the following way: $\boldsymbol{A} = U_1 \bowtie U_2 \bowtie \cdots \bowtie U_{d-1} \bowtie U_d$. The transpose $\boldsymbol{A}'$ of $\boldsymbol{A}$ is equal to the rank core product of the same cores, their blocks being transposed. If we consider another tensor $\boldsymbol{B} = V_1 \bowtie \cdots \bowtie V_d$ of the same mode size, then a linear combination of $\boldsymbol{A}$ and $\boldsymbol{B}$ can be written in the following way:

$$\alpha \boldsymbol{A} + \beta \boldsymbol{B} = \begin{bmatrix} U_1 & V_1 \end{bmatrix} \bowtie \begin{bmatrix} U_2 & \\ & V_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} U_{d-1} & \\ & V_{d-1} \end{bmatrix} \bowtie \begin{bmatrix} \alpha U_d \\ \beta V_d \end{bmatrix};$$

and the tensor product of $\boldsymbol{A}$ and $\boldsymbol{B}$, as $\boldsymbol{A} \otimes \boldsymbol{B} = U_1 \bowtie \cdots \bowtie U_d \bowtie V_1 \bowtie \cdots \bowtie V_d$.

Also, every matrix A may be regarded as a core of rank 1×1, and then the rank core product coincides with the Kronecker (tensor) product when applied to such cores.

Explicit rank reduction. Let us consider unfoldings $\boldsymbol{A}^{(k)}$ of $\boldsymbol{a}$ from (1.4), which are obtained from $\boldsymbol{a}$ by reshaping, indices $1, \dots, k$ and $k+1, \dots, d$ composing the row and column indices, respectively,

$$\boldsymbol{A}^{(k)}{}_{i_1 \dots i_k;\, i_{k+1} \dots i_d} = \boldsymbol{a}_{i_1 \dots i_d}. \tag{2.2}$$

Note that for every $k = 1, \dots, d-1$ equality (1.4) implies a low-rank representation of $\boldsymbol{A}^{(k)}$ of matrix rank r_k. Conversely, by representing *matrices* $\boldsymbol{A}^{(1)}, \dots, \boldsymbol{A}^{(d-1)}$ with ranks $r_1, \dots, r_d$ we obtain a TT decomposition (1.4) of $\boldsymbol{a}$ with *TT ranks* $r_1, \dots, r_{d-1}$ [32, Theorem 2.1] (in particular, the TT ranks of a vector itself are exactly the matrix ranks of its unfoldings). Consequently, the reduction of the ranks of a TT decomposition may be apprehended as the reduction of the rank of a low-rank representation of $\boldsymbol{A}^{(k)}$, performed successively for all $k = 1, \dots, d-1$. And in order to remove a linear dependence from these representations, one may apply the standard transformations of rows and columns to the core matrices. Indeed, the rank core product inherits the basic properties of the Kronecker (tensor) product; for instance,

$$\begin{aligned} \begin{bmatrix} \alpha_1 U_1 & \beta_1 U_1 \\ \alpha_1 V_1 & \beta_1 V_1 \end{bmatrix} \bowtie \begin{bmatrix} \alpha_2 U_2 & \alpha_2 V_2 \\ \beta_2 U_2 & \beta_2 V_2 \end{bmatrix} &= \left(\begin{bmatrix} U_1 \\ V_1 \end{bmatrix} \bowtie \begin{bmatrix} \alpha_1 & \beta_1 \end{bmatrix} \right) \bowtie \left(\begin{bmatrix} \alpha_2 \\ \beta_2 \end{bmatrix} \bowtie \begin{bmatrix} U_2 & V_2 \end{bmatrix} \right) \\ &= \begin{bmatrix} U_1 \\ V_1 \end{bmatrix} \bowtie \left(\begin{bmatrix} \alpha_1 & \beta_1 \end{bmatrix} \bowtie \begin{bmatrix} \alpha_2 \\ \beta_2 \end{bmatrix} \right) \bowtie \begin{bmatrix} U_2 & V_2 \end{bmatrix} \\ &= (\alpha_1 \alpha_2 + \beta_1 \beta_2) \begin{bmatrix} U_1 \\ V_1 \end{bmatrix} \bowtie \begin{bmatrix} U_2 & V_2 \end{bmatrix} \end{aligned} \tag{2.3}$$

for any coefficients $\alpha_1, \beta_1, \alpha_2, \beta_2$ and blocks *or* subcores U_1, V_1, U_2, V_2 of proper ranks and mode sizes. Equality (2.3) illustrates the basic technique we routinely use throughout the paper.

The QTT blocks we use. We use the following 2×2-matrices as QTT blocks to describe the QTT structure of the matrices under consideration:

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

$$E = \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad F = \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}, \quad K = \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad L = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix}. \tag{2.4}$$

Another remark. Finally, by $A^{\otimes k}$, where k is a nonnegative integer, we mean a kth tensor power of A. For example, $I^{\otimes 3} = I \otimes I \otimes I$, and likewise for the rank core product operation "$\bowtie$."

3. The QTT structure of tridiagonal Toeplitz matrices. Let us apply the notation and technique introduced above to derive a low-rank QTT representation of a tridiagonal Toeplitz matrix.

LEMMA 3.1. *Assume that $l \geq 2$ and α, β, γ are numbers. Then the matrix*

$$\boldsymbol{A}^{(l)} = \begin{pmatrix} \alpha & \beta & & & \\ \gamma & \alpha & \ddots & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \alpha & \beta \\ & & & \gamma & \alpha \end{pmatrix}$$

of size $2^l \times 2^l$ has the following QTT representation of ranks $3, \dots, 3$:

$$\boldsymbol{A}^{(l)} = \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie (l-2)} \bowtie \begin{bmatrix} \alpha I + \beta J + \gamma J' \\ \gamma J \\ \beta J' \end{bmatrix}.$$

Proof. We use the recursive block structure

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

which holds for $2 \leq k \leq l$. Let us recast it with the use of the rank core product:

$$\boldsymbol{A}^{(k)} = \begin{bmatrix} I & J' & J \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{A}^{(k-1)} \\ \gamma J^{\otimes (k-1)} \\ \beta J'^{\otimes (k-1)} \end{bmatrix}.$$

With the trivial equalities $\gamma J^{\otimes k} = J \otimes \gamma J^{\otimes (k-1)}$ and $\beta J'^{\otimes k} = J' \otimes \beta J'^{\otimes (k-1)}$ this gives us

$$\begin{bmatrix} \boldsymbol{A}^{(k)} \\ \gamma J^{\otimes k} \\ \beta J'^{\otimes k} \end{bmatrix} = \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{A}^{(k-1)} \\ \gamma J^{\otimes (k-1)} \\ \beta J'^{\otimes (k-1)} \end{bmatrix}, \tag{3.1}$$

which holds for $k = 2, \dots, l$. Next we apply equality (3.1) to itself recursively:

$$\begin{aligned} \begin{bmatrix} \boldsymbol{A}^{(k)} \\ \gamma J^{\otimes k} \\ \beta J'^{\otimes k} \end{bmatrix} &= \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix} \bowtie \left(\begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{A}^{(k-2)} \\ \gamma J^{\otimes (k-2)} \\ \beta J'^{\otimes (k-2)} \end{bmatrix} \right) \\ &= \dots = \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J \\ & J & \\ & & J' \end{bmatrix}^{\bowtie (k-2)} \bowtie \begin{bmatrix} \boldsymbol{A}^{(1)} \\ \gamma J \\ \beta J' \end{bmatrix}, \end{aligned}$$

where $\boldsymbol{A}^{(1)} = \alpha I + \beta J + \gamma J'$. By considering $k = l$ and selecting the first row in the first core, we conclude the proof. ∎

COROLLARY 3.2. *Let $l \geq 3$. Then*

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

$$\mathbf{\Delta}_{DN}^{(l)} = \begin{bmatrix} I & J' & J & I_2 \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I_2 \end{bmatrix}^{\bowtie (l-2)} \bowtie \begin{bmatrix} 2I - J - J' \\ -J \\ -J' \\ -I_2 \end{bmatrix}.$$

Proof. The proof follows from Lemma 3.1 and the relation $\mathbf{\Delta}_{\mathrm{DN}}^{(l)} = \mathbf{\Delta}_{\mathrm{DD}}^{(l)} - I_2^{\otimes d}$. ∎

Note that the cores of the decomposition obtained in Lemma 3.1 are of rank 1×3, 3×3, and 3×1, and, thus, the decomposition has equal ranks $3, \ldots, 3$. Similarly, the QTT representation of $\mathbf{\Delta}_{\mathrm{DN}}^{(l)}$ is of ranks $4, \ldots, 4$. Decompositions of the tridiagonal one-dimensional mass matrices (1.3) are obtained in the very same way.

4. Multigrid prolongation and restriction matrices. Rectangular matrices of a similar structure may be treated in the same way. For example, let us consider the prolongation and restriction operations involved in a tensor-structured geometric multigrid method. If the mixed Dirichlet–Neumann boundary conditions are imposed and a discretization we described in the introduction is used, then the corresponding one-dimensional matrices are of the form

$$\boldsymbol{P}^{(l)} = \frac{1}{2} \begin{pmatrix} 1 & & & & \\ 2 & & & & \\ 1 & 1 & & & \\ & 2 & & & \\ & 1 & \ddots & & \\ & & \ddots & 1 & \\ & & \ddots & 2 & \\ & & & 1 & 1 \\ & & & & 2 \end{pmatrix} \quad \text{and} \quad \boldsymbol{R}^{(l)} = \frac{1}{2} \boldsymbol{P}^{(l)\prime}, \tag{4.1}$$

where $\boldsymbol{P}^{(l)}$ is of size $2^{l+1} \times 2^l$ (see, e.g., [2, section 6]). Then we may write

$$\begin{aligned} \boldsymbol{P}^{(l)} &= \begin{bmatrix} I & J' \end{bmatrix} \bowtie \begin{bmatrix} \boldsymbol{P}^{(l-1)} \\ \frac{1}{2} J^{\otimes (l-1)} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{bmatrix} \\ &= \cdots = \frac{1}{2} \begin{bmatrix} I & J' \end{bmatrix} \bowtie \begin{bmatrix} I & J' \\ & J \end{bmatrix}^{\bowtie (l-2)} \bowtie \begin{bmatrix} \begin{pmatrix} 1 \\ 2 \end{pmatrix} \\ \begin{pmatrix} 1 \\ 0 \end{pmatrix} \end{bmatrix}, \end{aligned} \tag{4.2}$$

which also implies that

$$\boldsymbol{R}^{(l)} = \frac{1}{4} \begin{bmatrix} I & J \end{bmatrix} \bowtie \begin{bmatrix} I & J \\ & J' \end{bmatrix}^{\bowtie (l-2)} \bowtie \begin{bmatrix} \begin{pmatrix} 1 & 2 \end{pmatrix} \\ \begin{pmatrix} 1 & 0 \end{pmatrix} \end{bmatrix}. \tag{4.3}$$

Equalities (4.2) and (4.3) present rank-$2, \ldots, 2$ QTT representations of the one-dimensional prolongation and restriction matrices and lead to decompositions of their multidimensional counterparts $\boldsymbol{P}^{(l_1, \ldots, l_d)} = \boldsymbol{P}^{(l_1)} \otimes \cdots \otimes \boldsymbol{P}^{(l_d)}$ and $\boldsymbol{R}^{(l_1, \ldots, l_d)} = \boldsymbol{R}^{(l_1)} \otimes \cdots \otimes \boldsymbol{R}^{(l_d)}$ with the same ranks.

5. The TT and QTT structure of the d-dimensional Laplace matrix. Let us consider the following Laplace-like matrix:

$$\begin{aligned}\boldsymbol{\mathcal{L}}^{(d)} &= M_1 \otimes R_2 \otimes R_3 \otimes \cdots \otimes R_{d-2} \otimes R_{d-1} \otimes R_d \\ &+ L_1 \otimes M_2 \otimes R_3 \otimes \cdots \otimes R_{d-2} \otimes R_{d-1} \otimes R_d \\ &+ \cdots + L_1 \otimes L_2 \otimes L_3 \otimes \cdots \otimes L_{d-2} \otimes M_{d-1} \otimes R_d \\ &+ L_1 \otimes L_2 \otimes L_3 \otimes \cdots \otimes L_{d-2} \otimes L_{d-1} \otimes M_d,\end{aligned} \tag{5.1}$$

where the matrices L_k, M_k, and R_k are of size $m_k \times n_k$, $1 \leq k \leq d$. This matrix, which we need later, is a slight generalization of the Laplace matrix (1.1).

LEMMA 5.1. *For any $d \geq 2$ the Laplace-like matrix $\boldsymbol{\mathcal{L}}^{(d)}$ allows the following rank-$2, \ldots, 2$ TT representation in terms of the blocks L_k, M_k, and R_k:*

$$\boldsymbol{\mathcal{L}}^{(d)} = \begin{bmatrix} L_1 & M_1 \end{bmatrix} \bowtie \begin{bmatrix} L_2 & M_2 \\ & R_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} L_{d-1} & M_{d-1} \\ & R_{d-1} \end{bmatrix} \bowtie \begin{bmatrix} M_d \\ R_d \end{bmatrix}.$$

Proof. By the definition (5.1),

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

for all $k \geq 2$. We may revise it in terms of the rank core product as follows:

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

and, similarly to the proof of Lemma 3.1, we write

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

and, by applying the latter equality to itself recursively, we see that

$$\begin{bmatrix} L_1 \otimes \cdots \otimes L_{k+1} & \boldsymbol{\mathcal{L}}^{(k+1)} \end{bmatrix} = \begin{bmatrix} L_1 & M_1 \end{bmatrix} \bowtie \begin{bmatrix} L_2 & M_2 \\ & R_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} L_{k+1} & M_{k+1} \\ & R_{k+1} \end{bmatrix}$$

for $1 \leq k \leq d-1$. Next we choose $k = d-1$ and select the second columns in both the sides, which completes the proof. $\square$

Once QTT decompositions of each of the one-dimensional matrices L_k, M_k, and R_k, $1 \leq k \leq d$, are available, they can be easily merged into a QTT decomposition of the d-dimensional operator $\boldsymbol{\mathcal{L}}^{(d)}$ with the help of Lemma 5.1. For the sake of simplicity, let us assume that $R = L$. Then a straightforward verification or a formal recursion in the number of virtual dimensions l prove the following lemma.

LEMMA 5.2. *For $l \geq 2$ assume that the QTT representations $L = U_1 \bowtie \cdots \bowtie U_l$ and $M = V_1 \bowtie \cdots \bowtie V_l$ are of ranks $p_1, \ldots, p_{l-1}$ and $q_1, \ldots, q_{l-1}$, respectively; then the following QTT decompositions hold true:*

$$\begin{aligned}\begin{bmatrix} L & M \\ & L \end{bmatrix} &= \begin{bmatrix} U_1 & V_1 & \\ & & U_1 \end{bmatrix} \\ &\bowtie \begin{bmatrix} U_2 & & \\ & V_2 & \\ & & U_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} U_{l-1} & & \\ & V_{l-1} & \\ & & U_{l-1} \end{bmatrix} \bowtie \begin{bmatrix} U_l & \\ & V_l \\ & U_l \end{bmatrix},\end{aligned} \tag{5.2}$$

where the QTT ranks are $2p_1+q_1,\ldots,2p_{l-1}+q_{l-1}$*; and*

$$\begin{bmatrix} L & M \end{bmatrix} = \begin{bmatrix} U_1 & V_1 \end{bmatrix} \bowtie \begin{bmatrix} U_2 & \\ & V_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} U_{l-1} & \\ & V_{l-1} \end{bmatrix} \bowtie \begin{bmatrix} U_l & \\ & V_l \end{bmatrix}, \tag{5.3}$$

$$\begin{bmatrix} M \\ L \end{bmatrix} = \begin{bmatrix} V_1 & \\ & U_1 \end{bmatrix} \bowtie \begin{bmatrix} V_2 & \\ & U_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} V_{l-1} & \\ & U_{l-1} \end{bmatrix} \bowtie \begin{bmatrix} V_l \\ U_l \end{bmatrix}, \tag{5.4}$$

where the QTT ranks are $p_1+q_1,\ldots,p_{l-1}+q_{l-1}$.

Moreover, if it happens that $U_k=V_k$ *for* $1\le k\le l-1$*, then* (5.2) *and* (5.3) *reduce to the following decompositions:*

$$\begin{bmatrix} L & M \\ & L \end{bmatrix} = \begin{bmatrix} U_1 & \\ & U_1 \end{bmatrix} \bowtie \begin{bmatrix} U_2 & \\ & U_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} U_{l-1} & \\ & U_{l-1} \end{bmatrix} \bowtie \begin{bmatrix} U_l & V_l \\ & U_l \end{bmatrix}, \tag{5.5}$$

$$\begin{bmatrix} L & M \end{bmatrix} = U_1 \bowtie U_2 \bowtie \cdots \bowtie U_{l-1} \bowtie \begin{bmatrix} U_l & V_l \end{bmatrix} \tag{5.6}$$

of QTT ranks $2p_1,\ldots,2p_{l-1}$ *and* $p_1,\ldots,p_{l-1}$*, respectively.*

Now we may combine Lemma 5.2 with the results on the QTT structure of one-dimensional factors in (1.1) and Lemma 5.1 to obtain QTT representations of the Laplace matrix.

Corollary 5.3. *For* $d\ge 3$ *and* $l_1,\ldots,l_d\ge 3$ *let us consider the FDM* d*-dimensional Laplace matrix* $\mathbf{\Delta}^{(l_1\ldots l_d)}$ *from* (1.1) *with* $\boldsymbol{S}_k^{(l_k)} = \mathbf{\Delta}_{DD}^{(l_k)}$ *and* $\boldsymbol{M}_k^{(l_k)} = \mathbb{I}_{2^{l_k}} = I^{\otimes l_k}$, $1\le k\le d$*. Then the following QTT representations hold true for the factors of* $\mathbf{\Delta}^{(l_1\ldots l_d)}$ *in Lemma* 5.1*:*

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

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

$$\begin{bmatrix} a_k\mathbf{\Delta}_{DD}^{(l_k)} \\ I^{\otimes l_k} \end{bmatrix} = \begin{bmatrix} I & J' & J & \\ & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I \end{bmatrix}^{\bowtie(l_k-3)}$$

$$\bowtie \begin{bmatrix} a_kI & a_kJ' & a_kJ \\ & a_kJ & \\ & & a_kJ' \\ \frac{1}{2}I & -\frac{1}{2}I & -\frac{1}{2}I \end{bmatrix} \bowtie \begin{bmatrix} 2I-J-J' \\ -J \\ -J' \end{bmatrix}.$$

The resulting QTT decomposition of $\mathbf{\Delta}^{(l_1\ldots l_d)}$ *has ranks*

$$3,\ldots,3,\mathbf{2},4,\ldots,4,\mathbf{2},\ldots\ldots,\mathbf{2},4,\ldots,4,\mathbf{2},4,\ldots,4,3,$$

where we emphasize in boldface the ranks of the separation of "real" ("physical") dimensions, not the virtual ones.

Proof. For a middle factor, we start with (5.2) and reduce the ranks:

$$\begin{bmatrix} I^{\otimes l_k} & a_k\mathbf{\Delta}_{\mathrm{DD}}^{(l_k)} \\ & I^{\otimes l_k} \end{bmatrix} = \begin{bmatrix} I & I & J' & J & \\ & & & & I \end{bmatrix}$$

$$\bowtie \begin{bmatrix} I & & & & \\ & I & J' & J & \\ & & J & & \\ & & & J' & \\ & & & & I \end{bmatrix}^{\bowtie (l_k-2)} \bowtie \begin{bmatrix} I \\ a_k\,(2I-J-J') \\ -a_kJ \\ -a_kJ' \\ I \end{bmatrix}$$

$$= \begin{bmatrix} I & J' & J & \\ & & & I \end{bmatrix} \bowtie \begin{bmatrix} I & J' & J & \\ & J & & \\ & & J' & \\ & & & I \end{bmatrix}^{\bowtie (l_k-2)} \bowtie \begin{bmatrix} I & a_k\,(2I-J-J') \\ & -a_kJ \\ & -a_kJ' \\ & I \end{bmatrix}.$$

By selecting the first row (the second column) in both the sides, we obtain the decomposition of the outermost left (resp., right) factor. In the case of the outermost right factor the last rank can be reduced from 4 to 3 similarly to (2.3). ∎

Remark 5.4. For the FEM d-dimensional Laplace matrix $\boldsymbol{\Delta}^{(l_1 \ldots l_d)}$ from (1.1) with $\boldsymbol{S}_k^{(l_k)} = \boldsymbol{\Delta}_{\mathrm{DD}}^{(l_k)}$ and $\boldsymbol{M}_k^{(l_k)} = \boldsymbol{M}_{\mathrm{DD}}^{(l_k)}$, $1 \le k \le d$, the extra assumption of Lemma 5.2 holds due to Lemma 3.1, and one obtains a QTT decomposition of ranks

$$3, \ldots, 3, \mathbf{2}, 6, \ldots, 6, \mathbf{2}, \ldots\ldots, \mathbf{2}, 6, \ldots, 6, \mathbf{2}, 6, \ldots, 6,$$

which can be reduced to

$$3, \ldots, 3, \mathbf{2}, 4, \ldots, 4, \mathbf{2}, \ldots\ldots, \mathbf{2}, 4, \ldots, 4, \mathbf{2}, 4, \ldots, 4, 3$$

in a way similar to how we do it in the proof of Corollary 5.3.

The decompositions of the Laplace matrix for the mixed Dirichlet–Neumann boundary conditions are obtained in a similar way.

Below we also come across a sum

$$\boldsymbol{\mathcal{M}}^{(d)} = \sum_{k=1}^{d} U_1 \bowtie \cdots \bowtie U_{k-1} \bowtie \Gamma_k \bowtie V_{k+1} \bowtie \cdots \bowtie V_d, \tag{5.7}$$

of d products of TT cores of arbitrary consistent rank and mode sizes, so that each of the summands and the sum itself are correctly defined. Note that (5.7) turns into (5.1) in case $U_k = \begin{bmatrix} L_k \end{bmatrix}$, $\Gamma_k = \begin{bmatrix} M_k \end{bmatrix}$, and $V_k = \begin{bmatrix} R_k \end{bmatrix}$, $1 \le k \le d$. We do not restrict $\boldsymbol{\mathcal{M}}^{(d)}$ 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 be a TT core (i.e., also depend on two rank indices). Still, Lemma 5.1 can be easily generalized to $\boldsymbol{\mathcal{M}}^{(d)}$.

LEMMA 5.5. *For any $d \ge 2$ the matrix $\boldsymbol{\mathcal{M}}^{(d)}$ allows the following rank-$2 \ldots 2$ TT representation in terms of the cores U_k, Γ_k, and V_k:*

$$\boldsymbol{\mathcal{M}}^{(d)} = \begin{bmatrix} U_1 & \Gamma_1 \end{bmatrix} \bowtie \begin{bmatrix} U_2 & \Gamma_2 \\ & V_2 \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} U_{d-1} & \Gamma_{d-1} \\ & V_{d-1} \end{bmatrix} \bowtie \begin{bmatrix} \Gamma_d \\ V_d \end{bmatrix}.$$

Proof. The proof follows the proof of Lemma 5.1 owing to the properties of the rank core product inherited from the matrix and Kronecker products: "$\otimes$" can be formally replaced with "$\bowtie$"; L_k, M_k, and R_k, with U_k, Γ_k, and V_k, respectively. ∎

6. The QTT structure of the inverse Laplace matrix in one dimension.

Proposition 6.1. *The inverses of matrices* $\mathbf{\Delta}_{DD}^{(l)}$ *and* $\mathbf{\Delta}_{DN}^{(l)}$ *from* (1.2) *are the following:*

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

where $n = 2^l$.

Proof. The proof follows from either explicit expressions of the Green's functions of the corresponding Sturm–Liouville problems (see [38]) or a direct verification. ∎

Lemma 6.2. *For any* $l \ge 2$ *it holds that*

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

Proof. According to Proposition 6.1, the inverse of the matrix $\mathbf{\Delta}_{\mathrm{DN}}^{(l)}$ has the following form:

$$\mathbf{\Delta}_{\mathrm{DN}}^{(l)}{}^{-1} = \begin{bmatrix} I & I_2 & J & J' \end{bmatrix} \bowtie \begin{bmatrix} \mathbf{\Delta}_{\mathrm{DN}}^{(l-1)^{-1}} \\ 2^{l-1} E^{\otimes (l-1)} \\ \boldsymbol{K}^{(l-1)'} \\ \boldsymbol{K}^{(l-1)} \end{bmatrix}, \quad \boldsymbol{K}^{(k)} = \begin{pmatrix} 1 & 2 & 3 & \cdots & 2^k \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ \vdots & \cdots & \cdots & \cdots & \vdots \\ 1 & 2 & 3 & \cdots & 2^k \end{pmatrix},$$

so that

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

for $2 \le k \le l$. Then we find that

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

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

The latter equality, applied to itself recursively, completes the proof. ∎

LEMMA 6.3. *Let $l \geq 2$ 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 $1 \leq k \leq l$. Then ${\mathbf{\Delta}_{DD}^{(l)}}^{-1}$ has a rank-$5,\ldots,5$ QTT representation ${\mathbf{\Delta}_{DD}^{(l)}}^{-1} = W_l \bowtie W_{l-1} \bowtie \cdots \bowtie W_2 \bowtie W_1$, which consists of the TT cores

$$W_l = \begin{bmatrix} I & \frac{1}{4}\xi_l I + \frac{1}{4}\zeta_l P & \xi_l I - \zeta_l P & -\xi_l K & \zeta_l L \end{bmatrix},$$

$$W_k = \begin{bmatrix} I & \frac{1}{4}\xi_k I + \frac{1}{4}\zeta_k P & \xi_k I - \zeta_k P & -\xi_k K & \zeta_k L \\ & 2E & & & \\ & 2\eta_k^2 F & 2\xi_k^2 E & 2\xi_k\eta_k K & \xi_k\eta_k L \\ & 4\eta_k K & & 2\xi_k E & \\ & -4\eta_k L & & & 2\xi_k E \end{bmatrix}, \quad 2 \leq k \leq l-1,$$

$$W_1 = \begin{bmatrix} \frac{1}{3}(I+E) \\ 2E \\ \frac{1}{18}F \\ \frac{2}{3}K \\ -\frac{2}{3}L \end{bmatrix}.$$

Proof. Let $Q^{(k)}$ be a $2^k \times 2$-matrix comprising the columns 2^{k-1} and $2^{k-1}+1$ of $I^{\otimes k}$, and $D^{(k)} = I \otimes \mathbf{\Delta}_{\mathrm{DD}}^{(k-1)}$. Then from (1.2) it follows that $\mathbf{\Delta}_{\mathrm{DD}}^{(k)} = I \otimes \mathbf{\Delta}_{\mathrm{DD}}^{(k-1)} - Q^{(k)}\left(\begin{smallmatrix} 0 & 1 \\ 1 & 0 \end{smallmatrix}\right){Q^{(k)}}'$, and, by the Sherman–Morrison–Woodbury formula [12, p. 51],

$$\begin{aligned} {\mathbf{\Delta}_{\mathrm{DD}}^{(k)}}^{-1} &= I \otimes {\mathbf{\Delta}_{\mathrm{DD}}^{(k-1)}}^{-1} + A^{(k)}, \quad \text{where} \\ A^{(k)} &= {D^{(k)}}^{-1} Q^{(k)} B^{(k)} {Q^{(k)}}' {D^{(k)}}^{-1}, \\ B^{(k)} &= \left(\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}^{-1} - {Q^{(k)}}' {D^{(k)}}^{-1} Q^{(k)} \right)^{-1}, \end{aligned} \tag{6.1}$$

${D^{(k)}}^{-1} = I \otimes {\mathbf{\Delta}_{\mathrm{DD}}^{(k-1)}}^{-1}$. By Proposition 6.1, we may write

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

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 6.1, $2^{-k}x^{(k)}$ and $2^{-k}y^{(k)}$ are, respectively, the last and the first columns of ${\mathbf{\Delta}_{\mathrm{DD}}^{(k)}}^{-1}$; $2^{-k}{x^{(k)}}'$ and

$2^{-k}y^{(k)'}$ are rows. Thus,

$$A^{(k)} = \frac{1}{2^{k-1}} \left(\begin{array}{c|c} x^{(k-1)}x^{(k-1)'} & \zeta_k x^{(k-1)}y^{(k-1)'} \\ \hline \zeta_k y^{(k-1)}x^{(k-1)'} & y^{(k-1)}y^{(k-1)'} \end{array} \right). \tag{6.2}$$

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

$$\begin{aligned} x^{(k)}x^{(k)'} &= \frac{1}{4}e^{(k)}e^{(k)'} + \frac{1}{2}\left(e^{(k)}z^{(k)'} + z^{(k)}e^{(k)'}\right) + z^{(k)}z^{(k)'}, \\ y^{(k)}y^{(k)'} &= \frac{1}{4}e^{(k)}e^{(k)'} - \frac{1}{2}\left(e^{(k)}z^{(k)'} + z^{(k)}e^{(k)'}\right) + z^{(k)}z^{(k)'}, \\ x^{(k)}y^{(k)'} &= \frac{1}{4}e^{(k)}e^{(k)'} - \frac{1}{2}\left(e^{(k)}z^{(k)'} - z^{(k)}e^{(k)'}\right) - z^{(k)}z^{(k)'}, \\ y^{(k)}x^{(k)'} &= \frac{1}{4}e^{(k)}e^{(k)'} + \frac{1}{2}\left(e^{(k)}z^{(k)'} - z^{(k)}e^{(k)'}\right) - z^{(k)}z^{(k)'}. \end{aligned} \tag{6.3}$$

The right-hand matrices have a simple recursive structure:

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

therefore

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

With the use of the rank core product, this can be revised as follows:

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

where the cores V_k, $k \geq 2$, are defined as

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

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

$$\frac{1}{2^k}\begin{bmatrix} e^{(k)}e^{(k)'} \\ z^{(k)}z^{(k)'} \\ e^{(k)}z^{(k)'} + z^{(k)}e^{(k)'} \\ e^{(k)}z^{(k)'} - z^{(k)}e^{(k)'} \end{bmatrix} = V_k \bowtie \cdots \bowtie V_2 \bowtie V_1, \quad V_1 = \begin{bmatrix} 2E \\ \frac{1}{18}F \\ \frac{2}{3}K \\ -\frac{2}{3}L \end{bmatrix}. \tag{6.4}$$

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 combine (6.2), (6.3), and (6.4):

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

The recursive application of (6.1) results in the following expression for ${\mathbf{\Delta}_{\mathrm{DD}}^{(l)}}^{-1}$:

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

Let $U_k = \begin{bmatrix} I \end{bmatrix}$, $1 \leq k \leq d$, $\Gamma_1 = [{\mathbf{\Delta}_{\mathrm{DD}}^{(1)}}^{-1}]$; then

$$\begin{aligned} {\mathbf{\Delta}_{\mathrm{DD}}^{(l)}}^{-1} &= U_l \bowtie U_{l-1} \bowtie U_{l-2} \bowtie \cdots \bowtie U_3 \bowtie U_2 \bowtie \Gamma_1 \\ &+ U_l \bowtie U_{l-1} \bowtie U_{l-2} \bowtie \cdots \bowtie U_3 \bowtie \Gamma_2 \bowtie V_1 \\ &+ \cdots \\ &+ U_l \bowtie \Gamma_{l-1} \bowtie V_{l-2} \bowtie \cdots \bowtie V_3 \bowtie V_2 \bowtie V_1 \\ &+ \Gamma_l \bowtie V_{l-1} \bowtie V_{l-2} \bowtie \cdots \bowtie V_3 \bowtie V_2 \bowtie V_1. \end{aligned}$$

Then, in accordance with Lemma 5.5, it can be represented as follows:

$${\mathbf{\Delta}_{\mathrm{DD}}^{(l)}}^{-1} = \begin{bmatrix} I & \Gamma_l \end{bmatrix} \bowtie \begin{bmatrix} I & \Gamma_{l-1} \\ & V_{l-1} \end{bmatrix} \bowtie \cdots \bowtie \begin{bmatrix} I & \Gamma_2 \\ & V_2 \end{bmatrix} \bowtie \begin{bmatrix} \Gamma_1 \\ V_1 \end{bmatrix},$$

which concludes the proof. ∎

The rank-$5, \ldots, 5$ representation given by Lemma 6.3 can be reduced to a decomposition of ranks $4, 5, \ldots, 5, 4$ by a simple, but rather technical, calculation.

7. Conclusion. We investigated the TT and QTT structure of the Laplace matrix (1.1). The general TT structure is presented in Lemma 5.1, Corollary 5.3 deals with the QTT structure of the FDM discretization, and Remark 5.4 relates to the FEM discretization in the case of the Dirichlet boundary conditions. These results imply that the corresponding ranks are bounded from above by small constants (2, 4, and 6, respectively) independent of d and l_k, $k = 1, \ldots, d$. We implemented the decompositions presented in this paper in MATLAB and examined them with the help of the *TT Toolbox* (publicly available at http://spring.inm.ras.ru/osel). Our experiments showed that the TT and QTT ranks given in Lemma 5.1, Corollary 5.3, and Remark 5.4 are sharp, and the corresponding decompositions cannot be reduced. Also, the rank estimate resulting from Lemma 5.1 conforms to the observations presented in [33, Table 7.1]. Regarding the QTT structure, other boundary conditions can be considered analogously.

The structure of the inverse Laplace matrix is a completely different issue. Its TT ranks depend on d and l and are generally high. The TT and QTT approximations of the inverse Laplace matrix can be obtained through the quadrature techniques suggested in [14, 10, 4]. Some observation on the QTT ranks are given in [20, Table 4.1]. Only in the case of a single dimension ($\mathbf{\Delta}^{(l_1)} = \mathbf{\Delta}^{(l_1)}_{\mathrm{DD}}$ or $\mathbf{\Delta}^{(l_1)} = \mathbf{\Delta}^{(l_1)}_{\mathrm{DN}}$) are the exact QTT ranks low (resp., 5 or 4) independently of l. The corresponding decompositions are given by Lemmas 6.3 and 6.2 and can be used for the fast solution (logarithmic in the number of degrees of freedom 2^l) of the Poisson equation. What is more interesting, the rank estimate obtained for ${\mathbf{\Delta}^{(l)}_{\mathrm{DD}}}^{-1}$ conforms to the theorem presented in [40]. It claims that the QTT ranks of the inverse of a band Toeplitz matrix of bandwidth s are bounded from above by $4s^2 + 1$. However, we have no explicit solution to the general problem of the QTT-structured inversion of a band Toeplitz matrix.

Having considered the tensor structure of certain matrices, we note that in many situations one is interested more in the low-rank structure of matrix-vector products, which is, in general, a very different issue. For instance, the Fourier matrix is full-rank in the QTT format [6, Theorem 1], while the QTT ranks (exact or approximate) of Fourier images may be remarkably low [34, 6]. Another, somewhat more artificial, illustration is given in [16, section 5].

In all, the particular TT and QTT representations obtained may be useful in numerical experiments on model problems. On the other hand, the notation and technique we introduce to deal with explicit QTT representations on paper proves to be useful for other tensors, which are related to particular algorithms: the presented approach was used in [17] to examine the low-rank QTT structure of multilevel Toeplitz matrices and propose a fast QTT-structured convolution algorithm.

8. Implementation. The QTT decompositions of the FDM discretization of the Laplace operator and, in one dimension, of its inverse, presented above, are now available through the functions `tt_qlaplace_dd`, `tt_qlaplace_dn`, `tt_qlaplacex_dd`, and `tt_qlaplacex_dn` of the TT Toolbox.

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