

# Tensor properties of multilevel Toeplitz and related matrices

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## Abstract

A general proposal is presented for fast algorithms for multilevel structured matrices. It is based on investigation of their tensor properties and develops the idea recently introduced by J. Kamm and J. G. Nagy in the block Toeplitz case. We show that tensor properties of multilevel Toeplitz matrices are related to separation of variables in the corresponding symbol, present analytical tools to study the latter, expose truncation algorithms preserving the structure, and report on some numerical results confirming advantages of the proposal.

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## 1 Introduction

Despite a remarkable progress in fast algorithms for structured matrices in the last decades, many challenging gaps remain, especially concerning multilevel

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structured matrices.

Multilevel matrices frequently arise in multidimensional applications, where sizes of matrices may be very large and fast algorithms become crucial. However, most of the well-known fast algorithms for structured matrices are designed for one-level structured matrices, where request for large sizes is certainly weaker. Unfortunately, the one-level algorithms are not easy to adapt to the multilevel case. This applies, for example, to the multilevel Toeplitz matrices: fast algorithms are well developed for the Toeplitz matrices but very thin on the ground for the two-level (multilevel) Toeplitz matrices. This is likely to reflect the fact that the fabulous Gohberg-Sementsul and related formulas [7,11,13,25,6] for the inverse matrices are obtained only in the one-level case.

The main purpose of this paper is investigation of interrelations between the multilevel structured matrices and tensor-product constructions with accent on the two-level matrices. Specifically, the goal is to design iterative algorithms that find the inverse of a multilevel matrix using the following ideas. First, we believe that structure in the inverse matrices in the multilevel case may appear through approximation by appropriately chosen matrices of “simpler” structure. In this regard, tensor-product constructions can be attractive because of the very simple inversion formula

$$(A^1 \otimes \dots \otimes A^p)^{-1} = (A^1)^{-1} \otimes \dots \otimes (A^p)^{-1}.$$

Generally, inverses of multilevel matrices of low tensor rank may have an inverse that is close to a multilevel matrix of low tensor rank. Therefore in each iteration it makes sense to find a low tensor rank approximant. In the two-level case the latter low tensor rank approximants may be found by classical methods, e.g, SVD (in the more special Toeplitz case we can make function theoretic justifications). Finally, in the two-level Toeplitz case numerical results indicate that the approach is indeed promising.

Note that new ways for approximation of multilevel structured matrices are really in need for construction of preconditioners providing superlinear convergence of iterative methods. It was shown first in [21] that this can not be achieved when using any circulant-like preconditioner. Moreover, such a preconditioner cannot belong to standard matrix algebras [22]. More negative results in this line were recently obtained in [15]. All these results indicate that construction of efficient preconditioners could involve some sets of approximants other than matrix algebras, and our paper can be considered as a proposal of one alternative technique.

In Section 2 we recollect the framework for study of structures in multilevel matrices. Developing the ideas from [29], we introduce the notions of a structured class and tensor product of structured classes. The latter operation is used for construction of structured classes in multilevel matrices.

In Section 3 we study approximations of two-level matrices by sums of tensor products with the same structures of the factors. We discover here a somewhat surprising result that optimal Frobenius-norm approximations of low tensor rank for two-level matrices with certain structure on both levels *always* preserve the same one-level structures in the Kronecker factors (Theorem 3.2).

In Section 4 we show that the existence problem of tensor-product approximations for multilevel Toeplitz matrices reduces to approximate separation of variables in the corresponding generating function (symbol).

In Section 5 we present useful analytical tools to study the latter separation of variables. A general result is presented here for asymptotically smooth symbols (Theorem 5.2).

In Section 6 we present truncation algorithms for approximation of the inverse matrices, making a step towards better understanding of structure in the inverses to multilevel matrices.

In Section 7 we demonstrate some numerical results. We discover experimentally that the inverses to doubly Toeplitz matrices for various typical symbols possess low-tensor-rank approximations with the Kronecker factors of low displacement rank. In fact, we see from experiments that the so-called  $\varepsilon$ -displacement rank introduced in [2] is reasonably small for the Kronecker factors. From theoretical point of view, we are having thus a request for a rigorous formulation and proof. From algorithmical point of view, it suggests that we may look for different (and hopefully faster) truncation techniques in which this observation is adopted explicitly.

## 2 Structures in multilevel matrices

A general notion of multilevel matrix was introduced in [29]. Let  $A$  be a matrix of size  $M \times N$  with

$$M = \prod_{k=1}^p m_k, \quad N = \prod_{k=1}^p n_k.$$

Then, set

$$\mathbf{m} = (m_1, \dots, m_p), \quad \mathbf{n} = (n_1, \dots, n_p)$$

and introduce the index bijections

$$i \leftrightarrow \mathbf{i}(\mathbf{m}) = (i_1(\mathbf{m}), \dots, i_p(\mathbf{m})), \quad j \leftrightarrow \mathbf{j}(\mathbf{n}) = (j_1(\mathbf{n}), \dots, j_p(\mathbf{n}))$$

by the following rules:

$$i = \sum_{k=1}^p i_k \prod_{l=k+1}^p m_l, \quad j = \sum_{k=1}^p j_k \prod_{l=k+1}^p n_l,$$

$$0 \leq i \leq M - 1, \quad 0 \leq i_k \leq m_k - 1, \quad k = 1, \dots, p,$$

$$0 \leq j \leq N - 1, \quad 0 \leq j_k \leq n_k - 1, \quad k = 1, \dots, p.$$

Any entry  $a_{ij}$  of  $A$  can be pointed to by the index pair  $(\mathbf{i}(\mathbf{m}), \mathbf{j}(\mathbf{n}))$  revealing a certain hierarchical block structure in  $A$ . We will say that  $A$  is a  $p$ -level matrix and write

$$a_{ij} = a(\mathbf{i}, \mathbf{j}) \quad \text{or} \quad a_{ij} = a_{\mathbf{ij}},$$

freely replacing  $i$  by  $\mathbf{i}$  and  $j$  by  $\mathbf{j}$ . Introduce the truncated indices

$$\mathbf{i}_k = (i_1, \dots, i_k), \quad \mathbf{j}_k = (j_1, \dots, j_k).$$

Then  $a(\mathbf{i}_k, \mathbf{j}_k)$  will denote a block of level  $k$ . We will call  $\mathbf{m}$  and  $\mathbf{n}$  the *size-vectors* of  $A$ .

By definition,  $A$  itself is a single block of level 0. It consists of  $m_1 \times n_1$  blocks  $a(\mathbf{i}_1, \mathbf{j}_1)$ , these blocks being said to belong to the 1st level of  $A$ . At the same time,  $A$  consists of  $(m_1 m_2) \times (n_1 n_2)$  blocks  $a(\mathbf{i}_2, \mathbf{j}_2)$  of the 2nd level of  $A$ , and so on. It is important to note that each block of level  $k < p$  consists of  $m_{k+1} \times n_{k+1}$  blocks of level  $k + 1$ . Further on we chiefly assume that  $M = N$  and  $\mathbf{m} = \mathbf{n}$ .

Multilevel block partitionings are of interest only if the blocks of the levels exhibit some structure. For example,  $A$  is a  $p$ -level Toeplitz matrix if every block of level  $0 \leq k < p$  is a block Toeplitz matrix with the blocks of the next level. An equivalent definition is to say that  $a(\mathbf{i}, \mathbf{j})$  depends actually only on  $\mathbf{i} - \mathbf{j}$ . Thus, in the case of a  $p$ -level Toeplitz matrix we may write

$$A = [a(\mathbf{i} - \mathbf{j})].$$

A  $p$ -level matrix  $C$  is called a  $p$ -level circulant if every block of level  $0 \leq k < p$  is a block circulant matrix with the blocks of level  $k + 1$ . Equivalently,  $a(\mathbf{i}, \mathbf{j})$  depends only on

$$(\mathbf{i} - \mathbf{j})(\text{mod } \mathbf{n}) \equiv ((i_1 - j_1)(\text{mod } n_1), \dots, (i_p - j_p)(\text{mod } n_p)),$$

and one may write

$$C = [c((\mathbf{i} - \mathbf{j})(\text{mod } \mathbf{n}))].$$

Below we illustrate the structure of  $A$  and  $C$  in the case  $p = 2$  and  $\mathbf{n} = (3, 2)$ :

$$A = \left[ \begin{array}{cc|cc|cc} a(0,0) & a(0,-1) & a(-1,0) & a(-1,-1) & a(-2,0) & a(-2,-1) \\ a(0,1) & a(0,0) & a(-1,1) & a(-1,0) & a(-2,1) & a(-2,0) \\ \hline a(1,0) & a(1,-1) & a(0,0) & a(0,-1) & a(-1,0) & a(-1,-1) \\ a(1,1) & a(1,0) & a(0,1) & a(0,0) & a(-1,1) & a(-1,0) \\ \hline a(2,0) & a(2,-1) & a(1,0) & a(1,-1) & a(0,0) & a(0,-1) \\ a(2,1) & a(2,0) & a(1,1) & a(1,0) & a(0,1) & a(0,0) \end{array} \right],$$

$$C = \left[ \begin{array}{cc|cc|cc} c(0,0) & c(0,1) & c(2,0) & c(2,1) & c(1,0) & c(1,1) \\ c(0,1) & c(0,0) & c(2,1) & c(2,0) & c(1,1) & c(1,0) \\ \hline c(1,0) & c(1,1) & c(0,0) & c(0,1) & c(2,0) & c(2,1) \\ c(1,1) & c(1,0) & c(0,1) & c(0,0) & c(2,1) & c(2,0) \\ \hline c(2,0) & c(2,1) & c(1,0) & c(1,1) & c(0,0) & c(0,1) \\ c(2,1) & c(2,0) & c(1,1) & c(1,0) & c(0,1) & c(0,0) \end{array} \right].$$

A general description of structure in multilevel matrices can be introduced in the following way [30]. Denote by  $\mathbf{S}$  a sequence of linear subspaces  $\mathbf{S}^1, \mathbf{S}^2, \dots$  with  $\mathbf{S}^n$  being a subspace in the space of all  $n \times n$  matrices. Obviously,  $\mathbf{S}^n$  can be considered as a class of structured matrices of order  $n$ , and, if structures for individual  $n$  are worthy to consider as “traces” of a common structure, then  $\mathbf{S}$  is a reference to this common structure. Let us write  $A \in \mathbf{S}$  if there exists  $n$  such that  $A \in \mathbf{S}^n$ , and refer to  $\mathbf{S}$  as a *structured class*. To distinguish between different structured classes, we use different letters or lower indices (i.e.,  $S_\alpha$  and  $S_\beta$ ).

It is easy to see that Toeplitz or circulant matrices can be described exactly in this way. Moreover, diagonal, three-diagonal, banded matrices as well as matrices with a prescribed pattern of sparsity are all examples of the same description style.

Denote by  $\mathbf{S}_\alpha^n \otimes \mathbf{S}_\beta^m$  a subspace in the space of all two-level matrices with size-vector  $(n,m)$ , defined by the claim that

$$A = [a_{(i_1, i_2)(j_1, j_2)}] \in \mathbf{S}_\alpha^n \otimes \mathbf{S}_\beta^m$$

if and only if

$$A_{i_2 j_2}^2 \equiv [a_{(i_1, i_2)(j_1, j_2)}]_{i_1 j_1=0}^{n-1} \in \mathbf{S}_\alpha^n \quad \forall 0 \leq i_2, j_2 \leq m-1,$$

and

$$A_{i_1 j_1}^1 \equiv [a_{(i_1, i_2)(j_1, j_2)}]_{i_2 j_2=0}^{m-1} \in \mathbf{S}_\beta^m \quad \forall 0 \leq i_1, j_1 \leq n-1.$$

By  $\mathbf{S}_\alpha \otimes \mathbf{S}_\beta$  we mean a sequence  $\mathbf{S}_\alpha^n \otimes \mathbf{S}_\beta^m$  with the two indices  $n, m = 1, 2, \dots$ . We call  $\mathbf{S}_\alpha \otimes \mathbf{S}_\beta$  the *tensor product of structured classes*  $\mathbf{S}_\alpha$  and  $\mathbf{S}_\beta$ .

A natural generalization of the above-considered construction comes with the assumption that  $\mathbf{S}_\alpha$  is a sequence of subspaces  $\mathbf{S}_\alpha^n$  of multilevel matrices with size-vector  $\mathbf{n}$ . Then,  $\mathbf{S}_\alpha \otimes \mathbf{S}_\beta$  means a sequence of subspaces  $\mathbf{S}_\alpha^n \otimes \mathbf{S}_\beta^m$  of multilevel matrices with size-vector  $(\mathbf{n}, \mathbf{m})$ . The definition for  $\mathbf{S}_\alpha^n \otimes \mathbf{S}_\beta^m$  mimics the above definition with minor changes in the following way:

$$A = [a_{(\mathbf{i}_1, \mathbf{i}_2)(\mathbf{j}_1, \mathbf{j}_2)}] \in \mathbf{S}_\alpha^n \otimes \mathbf{S}_\beta^m$$

if and only if

$$\begin{aligned} A_{\mathbf{i}_2, \mathbf{j}_2}^2 &\equiv [a_{(\mathbf{i}_1, \mathbf{i}_2)(\mathbf{j}_1, \mathbf{j}_2)}]_{\mathbf{i}_1, \mathbf{j}_1 \in \mathcal{I}_n} \in \mathbf{S}_\alpha^n \quad \forall \mathbf{i}_2, \mathbf{j}_2, \\ A_{\mathbf{i}_1, \mathbf{j}_1}^1 &\equiv [a_{(\mathbf{i}_1, \mathbf{i}_2)(\mathbf{j}_1, \mathbf{j}_2)}]_{\mathbf{i}_2, \mathbf{j}_2 \in \mathcal{I}_m} \in \mathbf{S}_\beta^m \quad \forall \mathbf{i}_1, \mathbf{j}_1. \end{aligned}$$

Thus, having defined some classes of structured matrices  $\mathbf{S}_{\alpha_1}, \dots, \mathbf{S}_{\alpha_p}$  we can easily introduce a new class

$$\mathbf{S}_\gamma = \mathbf{S}_{\alpha_1} \otimes \dots \otimes \mathbf{S}_{\alpha_p}$$

of multilevel structured matrices. The number of levels for  $\mathbf{S}_\gamma$  is the sum of the numbers of levels for the classes involved. In line with these definitions, if  $\mathbf{T}$  stands for the Toeplitz matrices then  $\mathbf{T} \otimes \mathbf{T}$  means two-level Toeplitz matrices and, in the general case,

$$\mathbf{T}^p = \mathbf{T} \otimes \dots \otimes \mathbf{T} \quad (\mathbf{T} \text{ is repeated } p \text{ times})$$

means  $p$ -level Toeplitz matrices. Similarly, if  $\mathbf{C}$  stands for circulants then  $\mathbf{C}^p$  denotes  $p$ -level circulant matrices.

Also, we can easily describe a mixture of Toeplitz and circulant structures on different levels: for example,  $\mathbf{T} \otimes \mathbf{C}$  identifies block Toeplitz matrices with circulant blocks while  $\mathbf{C} \otimes \mathbf{T}$  designates block circulant matrices with Toeplitz blocks.

Another approach to construction of multilevel structured matrices exploits the notion of Kronecker (tensor) product. Consider matrices

$$A^k = [a_{i_k j_k}^k], \quad 0 \leq i_k, j_k \leq n_k - 1, \quad k = 1, \dots, p,$$

and define  $A = [a_{\mathbf{ij}}]$  as a  $p$ -level matrix of size-vector  $\mathbf{n} = (n_1, \dots, n_p)$  with the entries

$$a_{\mathbf{ij}} = a_{i_1 j_1}^1 a_{i_2 j_2}^2 \dots a_{i_p j_p}^p, \quad \mathbf{i} = (i_1, \dots, i_p), \quad \mathbf{j} = (j_1, \dots, j_p).$$

This matrix  $A$  is called the Kronecker (tensor) product of matrices  $A^1, \dots, A^p$  and denoted by

$$A = A^1 \otimes \dots \otimes A^p.$$

**Proposition.** *If  $A^k \in \mathbf{S}_{\alpha_k}$ ,  $k = 1, \dots, p$ , then*

$$A^1 \otimes \dots \otimes A^p \in \mathbf{S}_{\alpha_1} \otimes \dots \otimes \mathbf{S}_{\alpha_p}.$$

### 3 Optimal Kronecker approximations

Suppose that  $A$  is a two-level matrix of size-vector  $\mathbf{n} = (n_1, n_2)$  and try to approximate it by a sum of Kronecker products of the form

$$A_r = \sum_{k=1}^r A_k^1 \otimes A_k^2,$$

where the sizes of  $A_k^1$  and  $A_k^2$  are  $n_1 \times n_1$  and  $n_2 \times n_2$ , respectively. If  $A = A_r$  and  $r$  is the least possible number of the Kronecker-product terms whose sum is  $A$  then  $r$  is called the tensor rank of  $A$ .

Optimal approximations minimizing  $\|A - A_r\|_F$  can be obtained via the SVD algorithm due to the following observation [31]. Denote by

$$\mathcal{V}_{\mathbf{n}}(A) = [b_{(i_1, j_1)(i_2, j_2)}]$$

a two-level matrix with size-vectors  $(n_1, n_1)$  and  $(n_2, n_2)$  defined by the rule

$$b_{(i_1, j_1)(i_2, j_2)} = a_{(i_1, i_2)(j_1, j_2)}.$$

Then, as is readily seen, the tensor rank of  $A$  is equal to the rank of  $\mathcal{V}_{\mathbf{n}}(A)$ . Moreover,

$$\|A - A_r\|_F = \|\mathcal{V}_{\mathbf{n}}(A) - \mathcal{V}_{\mathbf{n}}(A_r)\|_F,$$

which reduces the problem of optimal tensor approximation to the problem of optimal lower-rank approximation.

In practice we are interested only in the cases when  $r \ll n_1, n_2$ , so low-rank approximations being exactly what we need to find for  $\mathcal{V}_{\mathbf{n}}(A)$  and then convert to low-tensor-rank approximations for  $A$  via  $\mathcal{V}_{\mathbf{n}}^{-1}$ . Computational vehicles can be the SVD or Lanzos bidiagonalization algorithm. The latter should be preferred if  $\mathcal{V}_{\mathbf{n}}(A)$  admits a fast matrix-by-vector multiplication procedure. However, a drawback of both vehicles in this direct approach is that  $\mathcal{V}_{\mathbf{n}}(A)$  does not have smaller sizes than  $A$ .

We propose an alternative approach that allows us to work with quite small matrices while explicitly preserving structure in the Kronecker factors. To introduce it, recall and adapt the proposal of [14] in the case  $A \in \mathbf{T} \otimes \mathbf{T}$ . In

this case  $\mathcal{V}_n(A) = [a_{(i_1-j_1)(i_2-j_2)}]$  has coinciding elements whenever  $i_1 - j_1 = \mu$  and  $i_2 - j_2 = \nu$ ,  $1 - n_1 \leq \mu \leq n_1 - 1$ ,  $1 - n_2 \leq \nu \leq n_2 - 1$ . It suggests to consider only independent free-parameter elements and take up a smaller matrix

$$W(A) = [a_{\mu\nu}], \quad 1 - n_1 \leq \mu \leq n_1 - 1, \quad 1 - n_2 \leq \nu \leq n_2 - 1. \quad (1)$$

Let us find a low-rank approximation

$$W(A) \approx W(A_r) \equiv \sum_{k=1}^r u^k (v^k)^\top,$$

$$u^k = [u_\mu^k], \quad 1 - n_1 \leq \mu \leq n_1 - 1, \quad v^k = [v_\nu^k], \quad 1 - n_2 \leq \nu \leq n_2 - 1,$$

then set

$$U^k = [u_{i_1-j_1}^k], \quad 0 \leq i_1, j_1 \leq n_1 - 1, \\ V^k = [v_{i_2-j_2}^k], \quad 0 \leq i_2, j_2 \leq n_2 - 1,$$

and consider the tensor approximation

$$A \approx A_r = \sum_{k=1}^r U^k \otimes V^k. \quad (2)$$

This approximation remains optimal in the subspace of interest and in appropriately chosen norm. If  $A \in \mathbf{T} \otimes \mathbf{T}$  then set

$$\|A\|_{\mathbf{T} \otimes \mathbf{T}} \equiv \|W(A)\|_F,$$

where  $W(A)$  is defined by (1). It is easy to see that  $A_r$  in (2) belongs to  $\mathbf{T} \otimes \mathbf{T}$  and

$$\|A - A_r\|_{\mathbf{T} \otimes \mathbf{T}} = \|W(A) - W(A_r)\|_F.$$

We can develop the above into quite a general construction. According to the definition (see Section 1),  $\mathbf{S}^n$  is a linear subspace in the space of all matrices of order  $n$ . Hence, any matrix  $P \in \mathbf{S}^n$  can be uniquely defined by some *free parameters* (which can be chosen, of course, as some entries of  $P$ ). The number of free parameters is equal to  $\dim \mathbf{S}^n$ . Let us denote by  $W(P)$  a vector-column of the free parameters for  $P$ . By the construction,  $P \leftrightarrow W(P)$  is a bijection, and we may write  $P = W^{-1}(W(P))$ . The definition of free parameters means that for any  $P \in \mathbf{S}^n$

$$P_{i_1 j_1} = \sum_{k=1}^p \alpha_{i_1 j_1}^k w_k, \quad (3)$$

where the coefficients  $\alpha_{i_1 j_1}$  are the same for all  $P \in \mathbf{S}^n$  and  $w_k$  are the free parameters. Therefore, any matrix  $P \in \mathbf{S}^n$  satisfies

$$\text{vec}(P) = A_S W(P), \quad (4)$$



where  $\text{vec}(P)$  transforms matrix into a vector taking column by column,  $A_S$  is a matrix of size  $n^2 \times p$ . We will call  $A_S$  a *structure-frame matrix*. Obviously, if (4) holds for some matrix  $W(P)$  then  $P \in S^n$ . The columns of  $A_S$  treated as  $n \times n$  matrices form a basis in the linear space  $\mathbf{S}^n$  ( $\text{rank } A_S = \dim S^n = p$ ).

Now, let  $A \in \mathbf{S}_1 \otimes \mathbf{S}_2$  for some structured classes  $\mathbf{S}_1$  and  $\mathbf{S}_2$ . If  $A$  is of size-vector  $\mathbf{n} = (n_1, n_2)$  then  $A \in \mathbf{S}_1^{n_1} \otimes \mathbf{S}_2^{n_2}$ . Let  $W_1$  and  $W_2$  denote the free-parameter bijections for  $\mathbf{S}_1^{n_1}$  and  $\mathbf{S}_2^{n_2}$ , respectively, with the structure-frame matrices

$$A_{\mathbf{S}_1} = [a_1^{\mathbf{S}_1}, \dots, a_p^{\mathbf{S}_1}], \quad A_{\mathbf{S}_2} = [a_1^{\mathbf{S}_2}, \dots, a_q^{\mathbf{S}_2}], \quad p = \dim S_1, \quad q = \dim S_2.$$

Then,

$$\begin{aligned} \mathbf{S}_1^{n_1} &= \text{span}\{W_1^{-1}(a_1^{\mathbf{S}_1}), \dots, W_1^{-1}(a_p^{\mathbf{S}_1})\}, \\ \mathbf{S}_2^{n_2} &= \text{span}\{W_2^{-1}(a_1^{\mathbf{S}_2}), \dots, W_2^{-1}(a_q^{\mathbf{S}_2})\}, \end{aligned} \tag{5}$$

and, obviously,

$$\mathbf{S}_1^{n_1} \otimes \mathbf{S}_2^{n_2} = \text{span}\{W_1^{-1}(a_k^{\mathbf{S}_1}) \otimes W_2^{-1}(a_l^{\mathbf{S}_2}), \quad k = 1, \dots, p, \quad l = 1, \dots, q\}.$$

Thus, the free-parameters defining  $A \in \mathbf{S}_1^{n_1} \otimes \mathbf{S}_2^{n_2}$  can be considered as the entries of a rectangular matrix of size  $p \times q$ . Denote this matrix by  $W(A)$  and write  $W = W_1 \otimes W_2$  to refer to the corresponding bijection  $A \leftrightarrow W(A)$ .

**Theorem 3.1** *Let  $A \in \mathbf{S}_1^{n_1} \otimes \mathbf{S}_2^{n_2}$ ,  $W_1$  and  $W_2$  be the free-parameter bijections for  $\mathbf{S}_1^{n_1}$  and  $\mathbf{S}_2^{n_2}$ , and  $W = W_1 \otimes W_2$ . Then  $\mathcal{V}_{\mathbf{n}}(A)$  can be written as*

$$\mathcal{V}_{\mathbf{n}}(A) = A_{\mathbf{S}_1} W(A) A_{\mathbf{S}_2}^T. \tag{6}$$

**Proof.** In line with (5), let

$$W_1^{-1}(a_k^{\mathbf{S}_1}) = [\alpha_{i_1 j_1}^k], \quad W_2^{-1}(a_l^{\mathbf{S}_2}) = [\beta_{i_2 j_2}^l].$$

Thus, if

$$A = [a_{(i_1 i_2)(j_1 j_2)}] \in \mathbf{S}_1^{n_1} \otimes \mathbf{S}_2^{n_2}$$

and

$$W(A) = [w_{kl}], \quad 1 \leq k \leq p, \quad 1 \leq l \leq q,$$

then

$$a_{(i_1 i_2)(j_1 j_2)} = \sum_{k=1}^p \alpha_{i_1 j_1}^k \sum_{l=1}^q \beta_{i_2 j_2}^l w_{kl} = \sum_{k=1}^p \sum_{l=1}^q \alpha_{i_1 j_1}^k \beta_{i_2 j_2}^l w_{kl},$$

which proves (6).

According to (6), a low-rank approximation for  $\mathcal{V}_{\mathbf{n}}(A)$  can be obtained via the SVD (singular value decomposition) of a matrix of the form  $A_{\mathbf{S}_1} W(A) A_{\mathbf{S}_2}^T$ . It can be done in the following way:

(1) Compute QR-factorization for matrices  $A_{S_1}$  and  $A_{S_2}$ :

$$A_{S_1} = Q_1 R_1, \quad A_{S_2} = Q_2 R_2.$$

(2) Compute SVD for matrix  $R_1 W(A) R_2^\top$ :

$$R_1 W(A) R_2^\top = U \Sigma V^\top.$$

(3) Then, the SVD of  $\mathcal{V}_n(A)$  reads

$$\mathcal{V}_n(A) = (Q_1 U) \Sigma (Q_2 V)^\top.$$

The cost of the QR factorization is  $O(pn^2 + qn^2)$  operations; it can be computed only once for a given structured class, on the *preprocessing stage*. Given a particular matrix  $A$  in this structured class, we have to compute the SVD of a smaller rectangular matrix of size  $p \times q$ .

Now we are ready to conclude that optimal tensor approximations to a two-level matrix from the tensor product of two structured classes can be obtained so that the Kronecker factors belong to the involved structured classes. Moreover and somewhat surprisingly, this applies to any Kronecker-product representation of the optimal approximations.

**Theorem 3.2** *Let  $A \in \mathbf{S}_1^{n_1} \otimes \mathbf{S}_2^{n_2}$ , and assume that*

$$A_r = \sum_{k=1}^r A_k^1 \otimes A_k^2, \quad (7)$$

*is the optimal approximation to  $A$  such that*

$$\|A - A_r\|_F = \min_{B_r} \|A - B_r\|_F$$

*over all matrices  $B_r$  of tensor rank  $r$ . Then  $A_k^1 \in \mathbf{S}_1^{n_1}$  and  $A_k^2 \in \mathbf{S}_2^{n_2}$ .*

**Proof.** Let  $A_r$  be of the form (7),  $u_k = \text{vec}(A_k^1)$ ,  $v_k = \text{vec}(A_k^2)$ . If  $A_r$  is the optimal approximation of tensor rank  $r$  to  $A$ , then  $\sum_{k=1}^r u_k v_k^\top$  is the optimal approximation of rank  $r$  to  $\mathcal{V}_n(A)$ . Consequently, the column-vectors  $u_k$  and  $v_k$  are linear combinations of the columns of  $Q_1 U$  and  $Q_2 V$ , respectively. Since  $Q_1 U = A_{S_1}(R_1^{-1}U)$  and  $Q_2 V = A_{S_2}(R_2^{-1}V)$ , the column-vectors  $u_k$  and  $v_k$  are linear combinations of the columns of  $A_{S_1}$  and  $A_{S_2}$ , which proves that  $A_k^1 = W_1^{-1}(u_k) \in \mathbf{S}_1$  and  $A_k^2 = W_2^{-1}(v_k) \in \mathbf{S}_2$ .

**Corollary.** *Assume that  $A \in \mathbf{S}_1^{n_1} \otimes \mathbf{S}_2^{n_2}$ . Then, any left singular vector  $u$  of  $\mathcal{V}_n(A)$  is such that  $W_1^{-1}(u) \in \mathbf{S}_1^{n_1}$ , and any right singular vector  $v$  of the same matrix is such that  $W_2^{-1}(v) \in \mathbf{S}_2^{n_2}$ .*

**Remark.** If a low-tensor-rank approximation is not optimal then its Kronecker factors may lose any structure. Fortunately, standard methods for computing low-rank approximations (in particular, incomplete cross approximation algorithm of [28]) seem to maintain structure.

When constructing a low-rank approximation to  $\mathcal{V}_n(A)$ , we may skip the QR factorization step and consider a low-rank approximation to  $W(A)$ :

$$W(A) \approx \sum_{k=1}^r u_k v_k^\top.$$

Then, the corresponding low-rank approximation to  $\mathcal{V}_n(A)$  is of the form

$$\mathcal{V}_n(A) \approx \sum_{k=1}^r (A_{S_1} u_k)(A_{S_2} v_k)^\top.$$

This approximation is not optimal in the Frobenius norm (in case of arbitrary  $A_{S_1}, A_{S_2}$ ) but it still preserve the structure in the Kronecker factors. It follows from (6) that  $\text{rank } \mathcal{V}_n(A) \leq \text{rank } W(A)$  and, moreover,

$$\|A - \tilde{A}_r\| \leq \|A - A_r\| \|A_{S_1}\| \|A_{S_2}\|,$$

which suggests to consider this approximation as *quasi-optimal*.

Theorem 3.2 obviously generalizes the corresponding result for the  $\mathbf{T} \otimes \mathbf{T}$  (doubly Toeplitz) matrices [14]. In a unifying way, it covers all most interesting classes of multilevel structured matrices.

**Example.** Consider two-level Toeplitz-plus-Hankel matrices. To find an optimal  $r$ -tensor-rank approximation  $A_r$  to  $A \in (\mathbf{T} + \mathbf{H}) \otimes (\mathbf{T} + \mathbf{H})$ , we should first specify the free parameters for the  $\mathbf{T} + \mathbf{H}$  class. We say that  $P = [p_{ij}]$  belongs to  $\mathbf{T} + \mathbf{H}$  if

$$p_{ij} = t_{i-j} + h_{i+j}, \quad i = 1, \dots, n, \quad j = 1, \dots, n.$$

Therefore, there are  $4n - 2$  free parameters and their natural selection is

$$W(P) = [t_{1-n}, \dots, t_{n-1}, h_2, \dots, h_{2n}].$$

The structure-frame matrix  $A_{\mathbf{T}+\mathbf{H}}$  is of size  $n^2 \times (4n - 2)$  and of the block form

$$A_{\mathbf{T}+\mathbf{H}} = \begin{bmatrix} A_{\mathbf{T}} & A_{\mathbf{H}} \end{bmatrix},$$

where  $A_{\mathbf{T}}$  and  $A_{\mathbf{H}}$  are structure-frame matrices for the Toeplitz and Hankel matrices, respectively. We can naturally index the rows of the involved structure-frame matrices by a pair of indices  $(i, j)$ ,  $i, j = 1, \dots, n$ . Then,

$$(A_{\mathbf{T}})_{(ij),s} = \delta_{i-j,s}, \quad (A_{\mathbf{H}})_{(ij),s} = \delta_{i+j,s}.$$

On the preprocessing stage, we are to construct the QR decomposition of  $A_{\mathbf{T}+\mathbf{H}}$  (we are not aware of explicit formulas and so do this numerically).

To illustrate the above theory, consider a simplified example of two-level Toeplitz-plus-Hankel matrix with size vector  $(p, p)$ :

$$A_{(i_1, i_2)(j_1, j_2)} = \frac{1}{\sqrt{(i_1 - j_1)^2 + (i_2 - j_2)^2 + 1}} + \frac{1}{\sqrt{(i_1 + j_1)^2 + (i_2 + j_2)^2}}.$$

As is readily seen, it is the sum of two matrices: one from  $\mathbf{T} \otimes \mathbf{T}$  and the other from  $\mathbf{H} \otimes \mathbf{H}$ . The structure-frame matrix  $W(A)$  has a block structure:

$$W(A) = \begin{pmatrix} W^{TT} & 0 \\ 0 & W^{HH} \end{pmatrix},$$

$$W_{ij}^{TT} = \frac{1}{\sqrt{i^2 + j^2 + 1}}, \quad i = -p + 1, \dots, p - 1, \quad j = 2, \dots, 2p,$$

$$W_{ij}^{HH} = \frac{1}{\sqrt{i^2 + j^2}}, \quad i = 2, \dots, 2p, \quad j = 2, \dots, 2p.$$

Table 6.1 shows the Frobenius-norm error of different approximations to  $A$  with tensor rank  $r$  obtained by two methods:

- optimal (based on the SVD of  $\mathcal{V}_n(A)$  with a preliminary QR-factorization step), and
- quasi-optimal (with the SVD of  $W(A)$  only).

The matrix size is  $n = p^2 = 1024$ .

Rank	3	7	10
Method	Relative error		
SVD of $\mathcal{V}_n(A)$	$6 \cdot 10^{-2}$	$3 \cdot 10^{-3}$	$4 \cdot 10^{-4}$
SVD of $W(A)$	$2 \cdot 10^{-1}$	$1 \cdot 10^{-2}$	$1 \cdot 10^{-3}$

**Table 6.1** Optimal and quasi-optimal approximations.

Our arguments can be extended over to the matrices with the number of levels greater than two. However, in this case such a powerful tool as the theory and algorithms for the singular value decomposition is not available (cf [1,3]). Thus, in practice we are interested to exploit the case of two levels as far as possible (cf [4,10,27]). Moreover, accurate low-rank approximation can be often obtained from picking up only a relatively small number of entries, which leads to very efficient practical algorithms (cf [8,9,28]).

## 4 Tensor properties and separability of symbols

Consider a family of multilevel Toeplitz matrices associated with the Fourier expansion of a generating function (symbol)  $F$ . In the case of  $p$  levels,  $F$  is a  $p$ -variate function

$$F(x_1, \dots, x_p) = \sum_{k_1=-\infty}^{\infty} \cdots \sum_{k_p=-\infty}^{\infty} f_{k_1, \dots, k_p} \exp(i(k_1 x_1 + \dots + k_p x_p)) \quad (8)$$

and the entries of  $A \in \mathbf{T}^p$  are given by

$$a_{(i_1, \dots, i_p)(j_1, \dots, j_p)} = f_{i_1 - j_1, \dots, i_p - j_p}. \quad (9)$$

By  $\|A\|_C$  we mean the maximal in modulus entry of  $A$ , and by  $\|A\|_{(1)}$  the 1-norm of Schatten (the sum of all singular values of  $A$ ).

**Theorem 4.1** *Assume that  $A \in \mathbf{T}^p$  is generated by*

$$F(x_1, \dots, x_p) \in L_1(\Pi), \quad \Pi = [-\pi, \pi]^p,$$

*according to (8), (9). Then, a separable approximation*

$$F_r(x_1, \dots, x_p) = \sum_{k=1}^r \phi_k^1(x_1) \cdots \phi_k^p(x_p)$$

*of the symbol  $F$  implies that  $A$  admits a tensor approximation*

$$A_r = \sum_{k=1}^r A_k^1 \otimes \cdots \otimes A_k^p$$

*with the entrywise error estimate*

$$\|A - A_r\|_C \leq \frac{1}{(2\pi)^p} \|F - F_r\|_{L_1(\Pi)}$$

*and the Schatten 1-norm estimate*

$$\frac{1}{N} \|A - A_r\|_{(1)} \leq \frac{2}{(2\pi)^p} \|F - F_r\|_{L_1(\Pi)}, \quad (10)$$

*where  $N$  is the order of  $A$ .*

**Proof.** It suffices to take into account the following:

$$\begin{aligned} & (A_r)_{i_1 - j_1, \dots, i_p - j_p} = \\ & \frac{1}{(2\pi)^p} \int_{-\pi}^{\pi} \cdots \int_{-\pi}^{\pi} F_r(x_1, \dots, x_p) \exp(-i((i_1 - j_1)x_1 + \dots + (i_p - j_p)x_p)) dx_1 \cdots dx_p = \end{aligned}$$

$$\frac{1}{(2\pi)^p} \sum_{k=1}^p \prod_{l=1}^p \left( \int_{-\pi}^{\pi} \phi_k^l(x_k) \exp(-i(i_k - j_k)x_k) dx_k \right). \quad \square$$

Note that more general forms of the inequality (10) were studied in [20], even with the optimal constants therein.

## 5 Analytical tools for approximate separability

Separation of variables is a topic of permanent interest in approximation theory (cf [1]). The purpose here is to relate the number of separable terms to the corresponding approximation accuracy. Obviously, the results depend on the smoothness properties of functions under query. In applications, a closer attention is obviously paid to functions with certain types of singularities.

Let us consider bivariate symbols  $F(x_1, x_2)$  on  $\Pi = [-\pi, \pi]^2$ . Then, one can apply general results for the so-called *asymptotically smooth* functions [26,27].  $F$  is called asymptotically smooth if it attains a finite value at any point except for  $(0, 0)$  and all its mixed derivatives satisfy the inequality

$$\left| \frac{\partial^{k_1} \partial^{k_2}}{(\partial x_1)^{k_1} (\partial x_2)^{k_2}} F(x_1, x_2) \right| \leq cd^{k_1+k_2} (k_1 + k_2)! (x_1^2 + x_2^2)^{(g-k_1-k_2)/2},$$

$$(x_1, x_2) \neq (0, 0),$$

for all sufficiently large nonnegative  $k_1, k_2$  with constants  $c, d > 0$  and a real-valued constant  $g$  independent of  $k_1$  and  $k_2$ . In our case it is sufficient to consider  $F$  only for  $(x_1, x_2) \in \Pi$ .

**Theorem 5.1** [27] *Assume that  $F$  is asymptotically smooth and arbitrary values  $0 < h, q < 1$  be chosen. Then for any  $m = 1, 2, \dots$  there exists a separable function  $F_r(x_1, x_2)$  with  $r$  terms such that*

$$r \leq (c_0 + c_1 \log h^{-1})m,$$

$$|F(x_1, x_2) - F_r(x_1, x_2)| \leq c_2 q^m (x_1^2 + x_2^2)^{q/2}, \quad (x_1, x_2) \notin [-h, h]^2,$$

where  $c_0, c_1, c_2$  are constants depending on  $q$  but not on  $m$ .

A direct corollary of this is the following

**Theorem 5.2** *Let  $A^n$  be a two-level Toeplitz matrix of size-vector  $\mathbf{n}$ , generated by asymptotically smooth symbol  $F$  such that*

$$\int_{-h}^h \int_{-h}^h |F(x_1, x_2)| dx_1 dx_2 = O(h^\tau), \quad \tau > 0,$$

and assume additionally that  $g > -4$ . Then, for any  $\varepsilon > 0$  there exists a tensor approximation  $A_r^n \in \mathbf{T} \otimes \mathbf{T}$  with  $r$  terms such that

$$r \leq C_1 \log^2 \varepsilon^{-1},$$

$$\|A^n - A_r^n\|_C \leq C_2 \varepsilon,$$

where  $C_1$  and  $C_2$  do not depend on  $\mathbf{n}$ .

**Proof.** Given  $\varepsilon > 0$ , choose  $h$  so that  $h^r \sim \varepsilon$  and chose  $m$  so that  $q^m \sim \varepsilon$ . Also, take into account that the function  $(x_1^2 + x_2^2)^{g/2}$  will be  $L_1$ -integrable on  $[-\pi, \pi]^2$  for  $g > -4$ . It remains to have recourse to Theorems 5.1 and 4.1.  $\square$

Applications also give rise to functions like, for instance,

$$F(x_1, x_2) = \Phi(\xi, \theta), \quad \xi = x_1^2, \quad \theta = x_2^2, \quad (11)$$

$$\Phi(\xi, \theta) = \frac{\exp(i\kappa(\xi + \theta)^\nu)}{(\xi + \theta)^\nu}, \quad 0 < \nu < 2, \quad \kappa \geq 0. \quad (12)$$

that are not asymptotically smooth. Note, by the way, that the derivatives of this  $F$  are not bounded. Acquisition of separable approximations in such cases requires some special tools. An excellent vehicle for many practical cases can be developed on the base of E. T. Whittaker's cardinal function ("a function of royal blood", by his words) and Sinc-functions [23]. This vehicle works good also for many asymptotically smooth functions.

Consider the case

$$F(x_1, x_2) = \mathcal{F}(\xi, \theta), \quad \xi = \left(\frac{x_1}{\pi}\right)^2, \quad \theta = \left(\frac{x_2}{\pi}\right)^2,$$

then  $0 \leq \xi \leq 1$  and  $0 \leq \theta \leq 1$ . The goal is approximate separation of variables  $\xi$  and  $\theta$ . The approach of [23] capitalizes on outstanding properties of functions of complex variable  $z$  analytic in a strip  $|\operatorname{Im}z| \leq d$ . Thus, the enterprize must begin with finding a way to make the initial problem fit into that framework. A useful possibility is the change of variable

$$\xi = \frac{1}{\cosh u}, \quad \cosh u = \frac{\exp(u) + \exp(-u)}{2}, \quad -\infty \leq u \leq +\infty,$$

with coming back to  $\xi$  in the end using the formula

$$u = \log(\xi^{-1}(1 + \sqrt{1 - \xi^2}))$$

or, alternatively,

$$u = \log(\xi^{-1}(1 - \sqrt{1 - \xi^2})).$$

In order to separate  $u$  and  $\theta$  we make use of the assumption that

$$g(u, \theta) \equiv \mathcal{F}\left(\frac{1}{\cosh u}, \theta\right)$$

can be considered as the trace of a function

$$g(z, \theta) \equiv \mathcal{F}\left(\frac{1}{\cosh z}, \theta\right)$$

that is analytic with respect to  $z$  in the strip  $|\operatorname{Im}z| \leq d$ . Moreover, the constructions of [23] require that  $g(z, \theta)$  enjoys as well the following properties:

$$\mathcal{J}(g, d, \theta) \equiv \int_{-\infty}^{\infty} (|g(u + id, \theta)| + |g(u - id, \theta)|) du < +\infty, \quad (13)$$

$$\lim_{u \rightarrow \infty} \int_{-d}^d (|g(u + iv, \theta)| + |g(-u + iv, \theta)|) dv = 0, \quad (14)$$

$$|g(u, \theta)| \leq c \exp(-p|u|), \quad c, p > 0. \quad (15)$$

Then  $g(u, \theta)$  can be approximated by

$$g_n(u, \theta) \equiv \sum_{k=-n}^n g(kh, \theta) S_{kh}(u), \quad (16)$$

where

$$S_{kh}(u) = \frac{\sin\left(\frac{\pi}{h}(u - kh)\right)}{\left(\frac{\pi}{h}(u - kh)\right)}, \quad (17)$$

and  $h$  can be chosen so that

$$|g(u, \theta) - g_n(u, \theta)| \leq P \exp(-Q\sqrt{n}), \quad P, Q > 0. \quad (18)$$

One can see that the interpolation formula (16) performs the wanted job of separation of  $u$  and  $\theta$ . All the same, one should be careful with the above construction because  $P$  and  $Q$  in the error estimate (18) *may depend* on  $\theta$ . Moreover, even  $d$  might appear to depend on  $\theta$ . Note also that the properties (13), (14), (15) are not taken for granted, they must be verified and are likely not to hold initially but appear only after some suitable transformation of the problem. Nevertheless, the approach can be adapted to successfully treat, for example, the function (11), (12).

Let us give more details pertinent to functions of the form (12). Take some  $\mu > 0$  and set up

$$\mathcal{F}(\xi, \theta) = \xi^\mu \Phi(\xi, \theta).$$

Then, consider

$$g(z, \theta) = \frac{1}{(\cosh z)^\mu} \Phi\left(\frac{1}{\cosh z}, \theta\right).$$

First of all, note that  $g(z, \theta)$  is analytic at any  $z$  such that

$$\cosh z \neq 0, \quad \frac{1}{\cosh z} + \theta \neq 0.$$



It is not difficult to see that  $g(z, \theta)$  is analytic in any strip  $|\operatorname{Im}z| \leq d < \pi/2$ . Verification of (13) results in the observation that

$$\mathcal{J}(g, d, \theta) = O\left(\frac{1}{\theta^\nu}\right).$$

Condition (14) is evidently fulfilled. Concerning (15), we find that it holds true with

$$c = O\left(\frac{1}{\theta^\nu}\right), \quad p = -\mu.$$

Consequently, the estimate (18) is valid. Some further details of theory in [23] can lead to the assertion that

$$P = O\left(\frac{1}{\theta^\nu}\right)$$

while  $Q$  is greater than  $\sqrt{\mu}$ .

## 6 Truncation algorithms for the inverse matrices

In many cases when  $A$  is a matrix (of order  $n$ ) of low tensor rank, it appears as well that  $A^{-1}$  is of low tensor  $\varepsilon$ -rank (which means that there exists  $F$  such that  $\|F\| \leq \varepsilon$  and the tensor rank of  $A^{-1} + F$  is much smaller than  $n$ ). In the next section we substantiate this claim by numerical experiments. But first consider some computational tools proving to be very efficient for computation of approximate inverses in the tensor format. The tools we discuss below are based on the Newton iteration.

In numerical linear algebra, the Newton iteration for the inversion of matrices is attributed to Hotelling [12] and Schulz [24]. It is of the form

$$X_i = 2X_{i-1} - X_{i-1}AX_{i-1}, \quad i = 0, 1, \dots, \quad (19)$$

where  $X_0$  is some initial approximation to  $A^{-1}$ . Since  $I - AX_i = (I - AX_{i-1})^2$ , the iterations (19) converge quadratically, provided that  $\|I - AX_0\| < 1$ . Each iteration requires two matrix multiplications. Since this is quite expensive for general matrices, the method is usually considered as a supplementary tool to refine some approximation which is obtained by a different method.

In case of certain structured matrices one Newton iteration can become cheap, which may allow us to start them from a very rough initial guess. Application of the Newton iteration to matrices with the so-called displacement structure was recently studied in [2,19]. To make computations feasible, in these applications each  $X_i$  is replaced by some approximation (truncation) of low displacement rank. Remarkably, it is proved in [19] that in this case, under some assumptions, the *truncated Newton iteration* still converges quadratically.

Now, let us assume that  $A$  is a sum of  $r$  tensor products. When applying (19), we perform two matrix multiplications at every iterative step. If the matrices to be multiplied are in the tensor format

$$M^1 = \sum_{i=1}^{r_1} A_i^1 \otimes B_i^1, \quad M^2 = \sum_{i=1}^{r_2} A_i^2 \otimes B_i^2,$$

then

$$M^1 M^2 = \sum_{i=1}^{r_1} \sum_{j=1}^{r_2} (A_i^1 A_j^2) \otimes (B_i^1 B_j^2).$$

Therefore, the matrix-by-matrix complexity is  $\mathcal{O}(r_1 r_2 n^{3/2})$ , which is much smaller than the standard  $\mathcal{O}(n^3)$  rule. While maintaining the tensor format during the Newton iteration, we observe, all the same, that the exact tensor rank can be squared at every iterative step, which slows down the algorithm. Fortunately, it might not apply to the tensor  $\varepsilon$ -rank. Thus,  $X_i$  is substituted with an appropriate approximation  $Y_i$  of smaller tensor rank so that

$$\|X_i - Y_i\|_F \leq \varepsilon \|X_i\|_F.$$

We will write

$$Y_i = R_\varepsilon(X_i).$$

Computation of  $Y_i$  reduces to a lower-rank approximation to a given low-rank matrix; this can be done efficiently by the SVD-based procedure called *recompression* [10,28].

***Truncated Newton iteration in the tensor format:***

$$X_i = R_\varepsilon(X_{i-1}(2I - AX_{i-1})), \quad i = 1, 2, \dots \quad (20)$$

The iterations are stopped when  $\|I - AX_i\|_F \leq \varepsilon$ .

Some theory behind the truncated Newton iteration in the tensor format has been recently proposed in [18]. In particular, if the tensor ranks of  $A$  and  $A^{-1}$  do not exceed  $r$  and the truncation retains  $r$  term on all steps, then the convergence is still quadratic. Moreover, if  $r$  is an upper estimate on the tensor  $\varepsilon$ -rank of  $A^{-1}$ , then the residual  $\|I - AX_i\|$  diminishes quadratically until it gets smaller than a certain quantity related to this  $\varepsilon$  [18].

Following [4], we speed up the matrix multiplications using a sparsification of the tensor factors via a discrete wavelet transform (for example, one of the Daubechies family; for problems related to irregular grids we advocate the wavelet-type transforms constructed in [17]). We get from  $A$  and  $X_0$  to the transformed matrices

$$\tilde{A} = (W \otimes W)A(W^\top \otimes W^\top), \quad \tilde{X}_0 = (W \otimes W)X_0(W^\top \otimes W^\top),$$

where  $W$  represents a one-dimensional wavelet transform, and then get from  $\tilde{A}$  and  $\tilde{X}_0$  to appropriate pseudosparsity matrices (nullifying the entries using some threshold). The pseudosparsity of the tensor factors helps to diminish the matrix-by-vector complexity. Numerical experiments confirm that the wavelet sparsification coupled with tensor approximations is a really powerful (and quite general) tool (an adequate theory is still to be thought of).

A very important problem is how to select an initial approximation  $X_0$ . It is well-known that, for an arbitrary matrix  $A$ , we can set

$$X_0 = \alpha A^\top,$$

and if  $\alpha < \sigma_{\min}^2(A)$  then

$$\|I - AX\|_2 < 1.$$

However, the Newton iteration may converge very slow in this case. We can be better off with the following scheme:

1. Set  $X_0 = \alpha A^\top$  and perform the Newton iteration with an accuracy  $\delta \gg \varepsilon$  to find a rough approximation  $M$  to the inverse. The  $\delta$ -truncated Newton iterations are expected to have a small complexity due to a small number (and pseudosparsity) of the tensor factors.
2. Use  $M$  as a new guess to start the Newton iteration with finer accuracy  $\varepsilon$ .

Of course, this scheme can be extended to three or more steps with relative errors  $\delta_1, \delta_2$ , and so on.

## 7 Numerical results

We illustrate the proposed technique on the following two-level (doubly) Toeplitz matrices with separable symbols:

- (1)  $F_1 = 2 - \cos x - \cos y$  (Discrete 5-point Laplacian on a uniform grid).
- (2) A family of symbols with increasing condition numbers:

$$G_r(x) = x^{2r} + y^{2r}, \quad r = 1, 2, 3.$$

The condition numbers of these matrices grow asymptotically as  $\mathcal{O}(n^{2r})$ .

- (3)  $F_2 = (2 - \cos x - \cos y)^2$ .

By Theorem 4.1, separability of the symbols implies that the corresponding doubly Toeplitz matrices are in the tensor format: with 2 terms for the symbols  $F_1, G_r$  and with 3 terms for  $F_2$ . Since the symbols are positive (except for one zero point  $x = y = 0$ ), the reciprocal symbols are approximately separable,

which suggests (yet does not prove in the rigorous sense) that the inverse matrices should be of low tensor rank. The latter is confirmed numerically (see the results in Table 7.1). Typical behavior of approximate tensor ranks when  $n$  increases is shown in Table 7.2 (for symbol  $F_1$ ).

Symbol	$F_1$	$G_1$	$G_2$	$G_3$	$F_2$
n	$128^2$	$128^2$	$128^2$	$64^2$	$32^2$
Tensor $\varepsilon$ -rank	9	9	10	7	12

**Table 7.1** Tensor  $\varepsilon$ -rank of the inverse matrices,  $\varepsilon = 10^{-4}$

n	$32^2$	$64^2$	$128^2$
Tensor $\varepsilon$ -rank	7	8	9

**Table 7.2** Dependence of the tensor  $\varepsilon$ -rank on  $n$ , symbol  $F_1$ ,  $\varepsilon = 10^{-4}$ .

We inverted the matrices using the algorithm from Section 6 with two levels of accuracy. For example, in the case of  $F_1$  and  $n = 16384$  we selected  $\delta = 10^{-3}$ . The first step of our two-step Newton's iteration consisted of 39 iterations and took 55.3 seconds. The final residue (in the Frobenius norm) was 1.6 (the initial residue was 15881). On the second step there were only 5 iterations but they took 77.4 seconds. The final residue was  $5.5 \cdot 10^{-6}$ .

Approximate sparsity of the tensor factors after the wavelet transform is confirmed by the fill-in ratio shown in Table 7.3 for symbol  $F_1$  (since the matrix generated by  $F_1$  is symmetric,  $U_i = V_i$ , therefore the filling of  $V_i$  is equal to the filling of  $U_i$ ).

Which factor	1	2	3	4	5	6	7
Fill-in ratio	0.5	0.59	0.60	0.59	0.62	0.63	0.63

**Table 7.3** Fill-in ratio for the first tensor factors,  $\varepsilon = 10^{-4}$ ,  $n = 16384$ .

Finally, we verify the following conjecture about structure of the tensor factors. If  $A = T_1 \otimes \dots \otimes T_r$  is the tensor product of nonsingular Toeplitz matrices, then  $A^{-1} = T_1^{-1} \otimes \dots \otimes T_r^{-1}$  is the tensor product of matrices with low displacement rank (the displacement rank of  $M$  is defined to be the rank of  $M - ZMZ^\top$ , where  $M = [\delta_{i,j+1}]$  [13], [11], [16]). We may conjecture that the displacement ranks of the factors pertaining to  $A^{-1}$  remain low also in the case when  $A$  is a sum of tensor products of Toeplitz matrices. To confirm our hypothesis, we present maximum and mean displacement  $\varepsilon$ -ranks for factors in tensor representation of  $A^{-1}$ . The figures below seem to support the conjecture.

Symbol	$F_1$	$G_1$	$G_2$	$G_3$	$F_2$
n	$128^2$	$128^2$	$128^2$	$64^2$	$32^2$
Max. displacement $\varepsilon$ -rank	16	15	13	10	6
Mean displacement $\varepsilon$ -rank	12.2	11.2	9	6	4

**Table 7.4** Displacement  $\varepsilon$ -ranks of the tensor factors for  $A^{-1}$ ,  $\varepsilon = 10^{-4}$ .

The main purpose of this paper is to present some alternative ideas and techniques. Our first experiments are encouraging, however more work needs to be done to develop efficient implementations. The work on these implementations is in progress, and it will be summarized elsewhere with a more detailed description, timings and details. Rigorous theory behind the given sketch of numerical results is also part of the on-going research. The use of these ideas could be a possible way for overcoming the negative results in [15], [22].

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