Hierarchical Kronecker Tensor-Product Approximations

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Abstract

The goal of this work is the presentation of some new formats which are useful for the approximation of (large and dense) matrices related to certain classes of functions and nonlocal (integral, integro-differential) operators, especially for high-dimensional problems. These new formats elaborate on a sum of few terms of Kronecker products of smaller-sized matrices (cf. [34, 35]). In addition to this we need that the Kronecker factors possess a certain data-sparse structure. Depending on the construction of the Kronecker factors we are led to so-called "profile-low-rank matrices" or hierarchical matrices (cf. [17, 18]). We give a proof for the existence of such formats and expound a gainful combination of the Kronecker-tensor-product structure and the arithmetic for hierarchical matrices.

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1 Introduction

Among the most challenging problems of numerical computations nowadays are those of high dimensions, for instance, integral or differential equations on $[0,1]^d$ for $d \gg 1$. Many standard approaches fail because of "the curse of dimensionality", those that survive are in some way linked with the idea of tensor-product constructions on all stages of the solution strategy, while "less structured" or "irregular" ingredients are relegated to some acceptably small dimensions (see, e.g., [3]).

What might this mean on the level of matrices? Given a matrix $A \in \mathbb{C}^{N\times N}$ of order $N = n^m$, we try to approximate it by a matrix A_r of the form

$$A_r = \sum_{k=1}^{r} V_k^1 \times \cdots \times V_k^m \;\approx\; A, \tag{1.1}$$

where the V_k^ℓ are matrices of order n, the number r of terms is rather small, and usually $m = d$. (However, m can be less than the spatial dimension d or even greater; cf. [34, 35].)

We recall that the Kronecker product operation "$\times$" is defined as follows: if $U = [u_{ij}]$, then the matrix $U \times V$ has the block-representation $[u_{ij}V]$; the row and column sizes of $U \times V$ are the products of the row and column sizes of U and V, respectively. We do not use brackets in (1.1), since the $\times$-operation is associative.

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¿From the practical point of view, we might be equally interested in approximations of the form

$$A_{r,D} = D + \sum_{k=1}^{r} V_k^1 \times \cdots \times V_k^m \;\approx\; A, \tag{1.2}$$

where D is a correction matrix with low complexity with respect of storage and matrix-vector multiplication (e.g., a diagonal matrix). Sometimes, the ansatz (1.2) is easier to get than (1.1); in this paper, however, it appears only as an intermediate step towards (1.1).

Advantages of replacing A with A_r are the following:

- *Data compression.* The storage for the V_k^ℓ matrices of (1.1) is only $\mathcal{O}(rn^2) = \mathcal{O}(rN^{2/m})$, while that for the original (dense) matrix A is $\mathcal{O}(N^2)$. The compression factor is $\mathcal{O}(rN^{2/m-2})$. Under certain assumptions we prove later that $r = \mathcal{O}(\log^\alpha N)$ for some $\alpha > 0$. It implies the compression factor $\mathcal{O}((\log^\alpha N)/N)$ for $m = 2$ and a *superlinear compression rate* $\mathcal{O}(N^{-1-p})$, $0 < p < 1 - 2/m$, for $m > 2$.
- *Matrix-by-vector complexity*[1]. The matrix-vector multiplication costs for A_r are also much less than those for A. Instead of $\mathcal{O}(N^2)$ operations for A, we now need only $\mathcal{O}(rn^{m+1}) = \mathcal{O}(rN^{1+1/m})$ operations. (This can be quite acceptable for moderate sizes, even possibly for all N of interest in a particular application, especially in the case of $m > 2$; [25].)

On the other side, there are possible disadvantages and concerns:

- The case $m = 2$ is well-studied concerning theory and algorithms for the construction of the Kronecker tensor-product approximations (see the discussion in Section 2), but this case is not satisfactory concerning the matrix-by-vector complexity. The latter is better in the case $m > 2$, but for $m > 2$ the construction of the Kronecker tensor-product approximations becomes a much more difficult problem that requires quite intricate algorithms (see [25]) and still needs an adequate theory (cf. [6]).
- The matrix-by-vector complexity with the Kronecker-tensor ansatz (1.1) is outperformed asymptotically by the almost[2] linear estimates which are typical for $\mathcal{H}$-matrices (see [17, 18, 19, 22, 23]) or the mosaic-skeleton method (cf. [31, 32, 33]) as well as the earlier well-known methods such as panel clustering [24], multipole [28, 30], and interpolation using regular or hierarchical grids (cf. [5, 27]).

In this paper we ponder on these concerns and propose a modification of the format (1.1) so that the disadvantages can be *entirely overcome.*

First, we avoid the above-mentioned theoretical and algorithmical difficulties of $m > 2$ by focusing on the case $m = 2$. Thus, we assume that A is of order $N = n^2$ and study approximations of the form

$$A_r = \sum_{k=1}^{r} U_k \times V_k \approx A, \tag{1.3}$$

where U_k and V_k are of order n. We refer to r as the *Kronecker (tensor) rank* of (this particular representation of) A_r.

Second, we show that U_k and V_k can possess the structure of general $\mathcal{H}$-matrices (cf. [17, 18]) or related, more specific structures depending on the method by which the Kronecker tensor-product approximation (1.3) is constructed. Altogether, this results in an almost linear matrix-by-vector complexity in n.

Obviously, approximations of the form (1.3) with additional structure of the Kronecker factors U_k, V_k cannot hold for arbitrary matrices. Our results apply mostly to a family of matrices associated with a function $f(x, y)$, $x, y \in \mathbb{R}^2$.

In the case of integral equations, this function f may be the kernel function of the integral operator. Then the *Galerkin* discretisation yields $A = [a_{ij}]_{1 \le i,j \le N}$ with

$$a_{ij} = \int_{K^i} \int_{K^j} f(x, y)\phi^i(x)\phi^j(y)dxdy, \qquad 1 \le i, j \le N, \tag{1.4}$$

[1] The term *matrix-by-vector complexity* is an abbreviation for the complexity of the matrix-vector multiplication.

[2] We call $\mathcal{O}(n \log^q n)$ for some fixed q *almost linear* in n.

where $\phi^1, \ldots, \phi^N$ are given ansatz and test functions belonging to a Cartesian grid with K^i being the support of ϕ^i. In the case of $x \in \mathbb{R}^2$, the basis functions $\phi^i(x)$ may be products $\varphi^{i_1}(x_1)\varphi^{i_2}(x_2)$.

In the *collocation* case, ansatz functions $\phi^1, \ldots, \phi^N$ and collocation points $x^1, \ldots, x^N$ are given, and the matrix becomes

$$a_{ij} = \int_{K^j} f(x^i, y)\phi^j(y)dy, \qquad 1 \le i, j \le N. \tag{1.5}$$

The *Nyström* discretisation may lead to the matrix

$$a_{ij} = f(x^i, y^j), \qquad 1 \le i, j \le N, \tag{1.6}$$

where $x^1 = y^1, \ldots, x^N = y^N$ are the grid nodes (provided that the quadrature weights are identical and f is smooth).

Remark 1.1 *Also the Galerkin matrix from (1.4) may take the form (1.6). Assume the situation* $\phi^i(x) = \varphi^{i_1}(x_1)\varphi^{i_2}(x_2)$ *with one-dimensional hat-functions* φ^ν *with* $\mathrm{supp}(\varphi^\nu) = [(\nu-1)\,h, (\nu+1)\,h]$ *at the nodal point* νh *(h: step size) and consider a periodic situation in* $x_1, x_2 \in [0, 1]$. *In the equidistant case, the ansatz functions satisfy* $\phi^\nu(x) = \phi^0(x - \nu h)$ *for* $\nu = (i_1, i_2)$. *Define the convolution*

$$f_h(x, y) := \int_0^1 \int_0^1 \int_0^1 \int_0^1 f(\xi, \eta)\phi^0(\xi - x)\phi^0(\eta - y)d\xi_1 d\xi_2 d\eta_1 d\eta_2.$$

Then the a_{ij} *from (1.4) coincide with* $a_{ij} = f_h(x^i, x^j)$. *Even if* f *has integrable singularities at* $\xi = \eta$, f_h *is continuous, so that the evaluation in* $a_{ij} = f_h(x^i, x^j)$ *makes sense.*

Surprisingly, there are also interesting examples of (1.4) with a smooth function f. The choice $x^k := y^k := \sqrt{2\pi/N}(k-1)$ and $f(x, y) := \exp(\mathrm{i}xy))$ leads to the matrix of the discrete Fourier transform.

In the integral equation context, in particular, in BEM applications, typical examples of f are the following *volume/single-layer potentials*:

$$f(x, y) = \log|x - y| \qquad \text{(2D Laplace equation)}, \tag{1.7a}$$

$$f(x, y) = \frac{1}{|x - y|} \qquad \text{(3D Laplace equation)}, \tag{1.7b}$$

$$f(x, y) = H_0^{(1)}(\kappa|x - y|) \qquad \text{(2D Helmholtz equation)}, \tag{1.7c}$$

$$f(x, y) = \frac{\exp(\mathrm{i}\kappa|x - y|)}{|x - y|} \qquad \text{(3D Helmholtz equation)}, \tag{1.7d}$$

where $|x - y|$ is the Euclidean distance between the points x and y and, in the last two formulae, κ is the so-called wave number; $H_0^{(1)}$ is the zero-order Hankel function of the first kind, and $\mathrm{i} = \sqrt{-1}$. We remark that (1.7a,b) are asymptotically smooth functions (for a definition see Section 4), while (1.7c,d) do not belong to this class.

It should be emphasised once more that our constructions require certain assumptions on the function f as well as on the basis functions and grids. Nevertheless, we are able to cover all the above-mentioned examples. Restrictions pertaining to the grids will be discussed later.

Let A be the Galerkin matrix from (1.4) associated with a sufficiently smooth function $f(x, y)$ with possible singularity at $x = y$. In this paper we address the following main issues:

- *Accuracy estimates.* Given a prescribed error bound $\varepsilon > 0$, we want to have a sufficiently small r (Kronecker rank) in (1.3) such that

  $$\|A - A_r\| \le \varepsilon\|A\|, \tag{1.8}$$

  where the norm is usually chosen as entry-wise maximum: $\|A\|_C := \max\{|A_{ij}| : 1 \le i, j \le N\}$. (As a matter of fact, in most cases we are able to provide entry-wise error estimates.) An important question is how r depends on ε and N. Our findings in this respect can be treated as "existence theorems" proving the existence of approximations with certain bounds on r and the error ε (cf. §3, 4).

- *Complexity estimates.* If $r = \mathcal{O}(\log^q N)$, then we already enjoy an almost linear amount of storage, so that the main topic of the investigations is the matrix-by-vector complexity. We propose an $\mathcal{H}$-matrix format for the Kronecker factors in (1.3) and prove the corresponding "existence theorems" in which we inquire into the dependence of the complexity upon ε and N.

- *Assumptions on $f(x, y)$ and the Galerkin basis functions.* Basically, $f(x, y)$ is supposed to be translation invariant and "smooth" off the diagonal $x \neq y$, while the Galerkin basis functions are assumed to be of the tensor-product structure.

The first "existence theorems" for the Kronecker tensor-product approximations are proposed in [34, 35]. Under certain assumptions, these results are of the form (in the case $m = 2$)

$$r = \mathcal{O}(\log^2 \varepsilon^{-1}), \quad \|A - A_r\|_C = \mathcal{O}(\varepsilon), \tag{1.9}$$

which leads to the matrix-by-vector compexity of the order $O(rN^{3/2})$. However, one needs to find a way to reduce the matrix-by-vector complexity for this theory to become really attractive for practice. One idea to this end is a combination of the Kronecker-product approximation with a further sparsification of the Kronecker factors by the discrete wavelet transform (see [7]). In this paper we propose a different approach making use of recent techniques developed for $\mathcal{H}$-matrices.

The proof of "existence theorems" in [34] reduces the problem of the Kronecker tensor-product approximation $A_r \approx A$ to the construction of *separable approximations* of a function F (cf. §2.1) defined on a rectangle with the only singularity at the origin. The identical problem appeared in the study of weakly admissible clusters in the theory of $\mathcal{H}$-matrices (see [22]). A separable approximation of F with r terms will lead to a Kronecker tensor-product approximation of the matrix with Kronecker rank r. The interior structure of the Kronecker factors will however depend on the method by which they are constructed.

In our paper, the main approach to the approximation of F is based on a global approximation (cf. §3), e.g., by the so called Sinc functions (cf. [22, 29]). It leads to the result

$$r = \mathcal{O}(\log \varepsilon^{-1} \cdot \log\log \varepsilon^{-1}), \quad \|A - A_r\|_C = \mathcal{O}(\varepsilon). \tag{1.10}$$

In the case of asymptotically smooth kernel function f the corresponding result (1.9) is weaker than (1.10). In this case the approximation of F uses conventional piecewise polynomial expansions on a family of hierarchically refined subdomains (cf. the standard theory of $\mathcal{H}$-matrices).

The most significant observation is that using the Sinc approximations both matrices U_k and V_k can be obtained in the format of $\mathcal{H}$-matrices (this might indicate that the Sinc method is a rather helpful approximation tool). This data-sparse structure of the Kronecker factors results in an almost linear storage and matrix-by-vector complexity in n. Therefore, even for $m = 2$, we enjoy the same superlinear compression rate $\mathcal{O}(N^{-1-p})$ with $0 < p < 1/2$, that, otherwise, takes place for the ansatz (1.1) with $m > 2$. Note that the matrices U_k and V_k obtained by the algebraic SVD-based recompression method (cf. [22, 33]) lead directly to the $\mathcal{H}$-matrix structure. This is what we observe in our numerical experiments.

The remaining part of the paper is as follows. In §2 we begin with a general description of the Kronecker tensor-product approximation. In §3 we give a brief recollection of the essentials of the proof of the Sinc method (cf. [22]) and then continue with a detailed analysis of the structure of the corresponding Kronecker factors. In §4 we recall the standard construction of piecewise polynomial approximation of F and analyse the structure of the corresponding Kronecker factors. In the hierarchical approximation method, as usual in the $\mathcal{H}$-matrix theory, we assume f to be asymptotically smooth, while in the Sinc case we formulate our assumptions on f in terms of analyticity properties of F. The latter assumption seems to be more general. In particular, there are certain cases (e.g., the Helmholtz equation) for which the Sinc method works while piecewise polynomial approximation methods do not.

Then, we dwell upon further discussion and analysis of the assumptions under which estimates of the form (1.9) could hold. In §5 we show that our assumptions can be weakened in several respects:

- We may consider certain non-shift-invariant functions f.

- The domain of f may be different from a rectangle. For example, it can be a disc with a Cartesian-product grid in polar coordinates. It can be a torus or sphere as well.

- The grid must be logically equivalent to a rectangular grid, but may differ dramatically from such a grid, e.g., by a nonlinear change of coordinates.

Finally, we give conclusions and formulate some hypotheses.

2 Kronecker Products and Separable Approximations

2.1 General Description

Let $A = [a(i,j)]_{1\le i,j\le N}$ be a matrix of size $N \times N$ where $N = n^2$. Then, any row i and column j of A can be viewed as an $n \times n$ array with the FORTRAN-style ordering. For that purpose we use the bijection

$$i \leftrightarrow (i_1, i_2), \quad j \leftrightarrow (j_1, j_2), \qquad 1 \le i, j \le n^2, \quad 1 \le i_1, i_2,\ j_1, j_2 \le n. \tag{2.1}$$

defined by

$$i = i_1 + (i_2 - 1)n, \quad j = j_1 + (j_2 - 1)n, \qquad 1 \le i_1, i_2, j_1, j_2 \le n. \tag{2.2}$$

Accordingly, A can be indexed by $((i_1, i_2), (j_1, j_2))$:

$$a(i,j) = a(i_1, i_2; j_1, j_2). \tag{2.3}$$

If $A = U \times V$, then, using the notation (2.3) and assuming $U = [u(i_2, j_2)]$ and $V = [v(i_1, j_1)]$, we have

$$a(i,j) = u(i_2, j_2)v(i_1, j_1). \tag{2.4}$$

Vice versa, the two-dimensional arrays $u(i_2, j_2)$, $v(i_1, j_1)$ can be regarded as one-dimensional vectors. Denote the corresponding vector-columns by u and v.

In the case of the matrix A from (2.3), the rows are indexed by $i = (i_1, i_2)$, while the columns are indexed by $j = (j_1, j_2)$. Consider now a new matrix $\tilde{A}$, whose rows and columns are indexed by the respective pairs (i_1, j_1) and (i_2, j_2), and whose entries are $\tilde{a}(i_1, j_1; i_2, j_2) := a(i_1, i_2; j_1, j_2)$. Then, the equation $A = U \times V$ holds if and only if $\tilde{A} = vu^T$. Note that by definition there is a bijective mapping $\mathcal{P}$ of the entries of A to those of $\tilde{A}$ (in this sense, $\tilde{A}$ is a rearranged version of A), but[3] there is *no* permutation matrix P with $\tilde{A} = PAP^\top$.

In the general case (cf. [38]),

$$A_r = \sum_{k=1}^{r} U_k \times V_k \quad \Longleftrightarrow \quad \mathcal{P}(A_r) := \tilde{A}_r = \sum_{k=1}^{r} v_k u_k^\top, \tag{2.5}$$

where

$$U_k = [u_k(i_2, j_2)]_{1\le i_2, j_2 \le n}, \qquad V_k = [v_k(i_1, j_1)]_{1\le i_1,\ j_1 \le n}.$$

The correspondence $\mathcal{P} : A \mapsto \tilde{A}$ is a bijective mapping preserving the Frobenius norm. Note that the number r of terms is identical on both sides of (2.5). On the left side, r was called the Kronecker rank, while on the right side $r = \operatorname{rank}(\tilde{A}_r)$ holds, provided that the v_k and u_k are both linearly independent. A trivial, but helpful conclusion is given in

Remark 2.1 *The problem to find a Kronecker tensor-product approximation A_r of A with hopefully small r, is identical to the problem of finding a low-rank approximation $\tilde{A}_r$ of $\tilde{A}$.*

Thus, theory and algorithms for the approximations to A by (1.3) are reduced to those for low-rank approximations to $\tilde{A}$. In the latter case, theory and algorithms are available, e.g., the well-established matrix tools such as SVD or the Lanczos bidiagonalisation method (cf. [13]) and also efficient recent techniques such as incomplete cross approximation (cf. [33]) or adaptive cross approximation (cf. [1]) substantiated by the matrix theory results of [12, 14] and interpolation arguments in the BEM context [1]. Notice that in our applications the typical structure of $\tilde{A}$ corresponds to the so-called weakly admissible blocks of the $\mathcal{H}$-matrix

[3]Here, by accident, A and $\tilde{A}$ are both of size $N \times N$. But in the case of $1 \le i_1, j_1 \le n_1$ and $1 \le i_2, j_2 \le n_2$, A is a square matrix of size $n_1 n_2 \times n_1 n_2$, whereas $\tilde{A}$ is rectangular of size $n_1^2 \times n_2^2$.

technique described in [22]. For this class of matrices, the corresponding generalisation of the adaptive cross approximation is based on a blockwise agglomeration process with a recompression (cf. [22]), that uses a hierarchical decomposition of the domain similar to that in Section 4.

Assuming (1.6) with some function $f(x,y)$ of the coordinates $x = (x_1, x_2)$ and $y = (y_1, y_2)$, we can reduce the question about low-rank approximations of $\tilde{A}$ to the question about an approximation of $f(x,y) = f(x_1, x_2; y_1, y_2)$ by the following *separable approximation* with small r:

$$f(x_1, x_2; y_1, y_2) \approx f_r(x_1, x_2; y_1, y_2) = \sum_{k=1}^{r} \Phi_k(x_1, y_1)\Psi_k(x_2, y_2). \tag{2.6}$$

Note that (2.6) does not separate the x- and y-variables, but instead we separate the first components of x and y from the second ones.

If f is shift-invariant, then we actually have

$$f(x_1, x_2; y_1, y_2) = F(\zeta, \eta) \tag{2.7}$$

with

$$\zeta = x_1 - y_1, \quad \eta = x_2 - y_2 \tag{2.8}$$

and consider *separable approximations* of the form

$$F(\zeta, \eta) \approx F_r(\zeta, \eta) = \sum_{k=1}^{r} \Phi_k(\zeta)\Psi_k(\eta). \tag{2.9}$$

We will refer to r as the *separation rank* (of this particular representation) of $F_r(\zeta, \eta)$.

A natural bridge between approximations of functions and of function-value matrices (1.6) is provided by the evaluation of the function values at some grids. In our case, the grid should be the Cartesian product of two one-dimensional grids (in a weakened form, this is assumed at least with respect to some appropriately chosen coordinates):

$$x^i = (x_1^{i_1}, x_2^{i_2}), \quad i \leftrightarrow (i_1, i_2). \tag{2.10}$$

(Note that the superscripts in $x_1^{i_1}$ are not exponents.) We assume also that the nodes of the one-dimensional grids are numbered in increasing order:

$$x_1^1 < \ldots < x_1^n, \qquad x_2^1 < \ldots < x_2^n. \tag{2.11}$$

Obviously, (2.6) and (2.10) imply immediately (1.3), (2.5) with

$$u_k(i_2, j_2) = \Psi_k(x_2^{i_2}, x_2^{j_2}), \qquad v_k(i_1, j_1) = \Phi_k(x_1^{i_1}, x_1^{j_1}). \tag{2.12}$$

In the collocation case (1.5) and the Galerkin case (1.4), we require that the test functions possess the following tensor-product properties:

$$\phi^i(x_1, x_2) = \hat{\phi}^{i_1}(x_1)\hat{\phi}^{i_2}(x_2), \quad i \leftrightarrow (i_1, i_2). \tag{2.13}$$

(To simplify the presentation, we use the same uni-variate functions in both dimensions.) Consequently, in the collocation case

$$\begin{aligned} u_k(i_2, j_2) &= \textstyle\int \Psi_k(x_2, y_2)\hat{\phi}^{j_2}(y_2)dy_2, \\ v_k(i_1, j_1) &= \textstyle\int \Phi_k(x_1, y_1)\hat{\phi}^{j_1}(y_1)dy_1, \end{aligned} \tag{2.14}$$

and in the Galerkin case

$$\begin{aligned} u_k(i_2, j_2) &= \textstyle\iint \Psi_k(x_2, y_2)\hat{\phi}^{i_2}(x_2)\hat{\phi}^{j_2}(y_2)dx_2dy_2, \\ v_k(i_1, j_1) &= \textstyle\iint \Phi_k(x_1, y_1)\hat{\phi}^{i_1}(x_1)\hat{\phi}^{j_1}(y_1)dx_1dy_1. \end{aligned} \tag{2.15}$$

Suppose that the support of $\hat{\phi}^\ell$ is the closed interval $[\mu^\ell, \nu^\ell]$, $\ell = 1, \ldots, n$. Later we will add the assumption that

$$\mu^1 \le \ldots \le \mu^n, \qquad \nu^1 \le \ldots \le \nu^n. \tag{2.16}$$

Now we have defined the vectors u_k, v_k in the right part of (2.5) as well as the matrices (Kronecker factors) U_k, V_k.

Sometime the following "trick" might help in the study of approximations (2.9): With an appropriate choice of uni-variate functions $\mathcal{F}(\zeta)$ and $\mathcal{G}(\eta)$ it might be easier to consider separable approximations for

$$F_0(\zeta,\eta) = \mathcal{F}(\zeta)F(\zeta,\eta)\mathcal{G}(\eta). \tag{2.17}$$

Suppose we have proved that

$$\max_{\zeta,\eta}\left|F_0(\zeta,\eta) - \sum_{k=1}^{r}\Phi_{0k}(\zeta)\Psi_{0k}(\eta)\right| \le \varepsilon. \tag{2.18}$$

Then we set

$$\Phi_k(\zeta) = \frac{\Phi_{0k}(\zeta)}{\mathcal{F}(\zeta)}, \qquad \Psi_k(\eta) = \frac{\Psi_{0k}(\eta)}{\mathcal{G}(\eta)}. \tag{2.19}$$

This results in

$$\|A - A_r\|_C \le \varepsilon \max_{i_1,i_2,j_1,j_2}\int\int\int\int\left|\frac{\hat\phi^{i_1}(x_1)\hat\phi^{i_2}(x_2)\hat\phi^{j_1}(y_1)\hat\phi^{j_2}(y_2)}{\mathcal{F}(x_1-y_1)\mathcal{G}(x_2-y_2)}\right| dx_1dx_2dy_1dy_2. \tag{2.20}$$

Note that we need take care for the integrals in (2.20) to exist. Below we shall make use of the following choice:

$$\mathcal{G}(\eta) = 1, \quad \mathcal{F}(\zeta) = |\zeta|^{\alpha_0}, \quad 0 < \alpha_0 < 1. \tag{2.21}$$

The transformation (2.17) can be used to weaken the singularity of F and facilitates the application of some available theory (cf. §3.1 and Examples 1 - 3 in §3.2).

The interest in the separable approximation (2.9) (resp. (2.18)) of F (resp. F_0) is due to

Remark 2.2 *The error $\|A - A_r\|$ is directly related to the error $\|F - F_r\|$ of the separable approximation (2.9) of F. In particular, there holds*

$$\|A - A_r\|_C \le C\|F - F_r\|_C.$$

Proof. The combination of Remark 2.1 and the above arguments (cf. (2.20)) proves the assertion. ∎

Now we see that the separation rank of (2.9) or (2.18)-(2.19) determines the Kronecker rank of A_r.

2.2 Approximate Arithmetic in the New Format

For practice, the most helpful approximation format among the formats presented in this paper is likely to be the Kronecker tensor-product representation with the Kronecker factors being $\mathcal{H}$-matrices. For brevity, let us call it the HKT format (**H**ierarchical **K**ronecker **T**ensor format).

More precisely, let us write $A \in \mathrm{HKT}(r,s)$ if A is the sum of r Kronecker products

$$A = \sum_{k=1}^{r} U_k \times V_k$$

such that each Kronecker factor U_k and V_k has a hierarchical block partitioning (uniform with respect to k) with blocks of rank at most s. As above, we assume that $A \in \mathbb{C}^{N\times N}$, $N = n^2$, and $U_k, V_k \in \mathbb{C}^{n\times n}$.

If $A \in \mathrm{HKT}(r,s)$, then its storage amount is $\mathcal{O}(rs\sqrt{N}\log N)$ and multiplication by a vector needs $\mathcal{O}(rsN\log N)$ operations (cf. Algorithm 4.4 and following remarks).

Matrix-by-vector complexity for special vectors. Assume that $x \in \mathbb{C}^N$ is of the form

$$x = \sum_{\ell=1}^{r_x} x_\ell^1 \times x_\ell^2, \qquad x_\ell^1, x_\ell^2 \in \mathbb{C}^n. \tag{2.22}$$

Then

$$Ax = \sum_{k=1}^{r}\sum_{\ell=1}^{r_x}(U_k x_\ell^1) \times (V_k x_\ell^2). \tag{2.23}$$

Consequently, A can be multiplied by such an x in $\mathcal{O}(r_x r s\sqrt{N}\log N)$ operations (the multiplication complexity is almost linear in $n=\sqrt{N}$, the size of U_k and V_k).

If x is not exactly of the form (2.22), it might (and quite frequently does) happen that within the allowed computation error it can be replaced by a vector of this form. Considering x (respectively Ax) as an $n\times n$ matrix and using recompression (cf. Section 3.4), we may sacrifice some accuracy in favour of reducing the number r_x of summands in (2.22) (respectively in (2.23)). In principle, we can try this for all the vectors arising during some computational process (for example, in PCG or GMRES iterations).

Matrix-by-matrix complexity. If $A, B \in \mathrm{HKT}(r,s)$, then in general $AB \notin \mathrm{HKT}(r,s)$. However, the assumption

$$A=\sum_{k=1}^{r} U_k^A \times V_k^A, \quad B=\sum_{\ell=1}^{r} U_\ell^B \times V_\ell^B, \qquad U_k^A, V_k^A, U_\ell^B, V_\ell^B \in \mathbb{C}^n, \tag{2.24}$$

implies that

$$AB=\sum_{k=1}^{r}\sum_{\ell=1}^{r}(U_k^A U_\ell^B)\times(V_k^A V_\ell^B). \tag{2.25}$$

It can be proved that the matrices $U_k^A U_\ell^A$ and $V_k^A V_\ell^B$ possess the same hierarchical partitioning as the initial factors in (2.24) with blocks of possibly larger rank $s_{AB}\geq s$, bounded, nevertheless, by

$$s_{AB}=\mathcal{O}(s\log N).$$

Thus, $AB\in\mathrm{HKT}(r^2,s_{AB})$ with $s_{AB}=\mathcal{O}(s\log N)$. Keeping the same s for the $\mathcal{H}$-format approximations of $U_k^A U_\ell^B$ and $V_k^A V_\ell^B$, we can approximate AB by some matrix $C\in\mathrm{HKT}(r^2,s)$, the construction of C costs $\mathcal{O}(r^2 s^2\sqrt{N}\log N)$; cf. [16, 17, 22]. Using recompression, we can also try to reduce the number of the Kronecker products. However, now it is a nontrivial problem since the Kronecker factors $U_k^A U_\ell^B$ and $V_k^A V_\ell^B$ are represented in the $\mathcal{H}$-format.

Computation of the inverse matrix. For a class of elliptic operators, an efficient method to construct the HKT-approximation to the inverse operator was developed in [11].

In the general case, a construction of the HKT-formatted inverse can be based on the Newton method or on the block Gauss elimination (giving rise to the so-called Frobenius formulae). In implementation, either approach reduces to matrix-matrix-multiplications which can be performed in the approximate and fast way as it is shown above. A detailed presentation of the corresponding algorithms is beyond the scope if this paper. The overall complexity is of the desired order only if the recompression after each matrix-matrix-multiplication does not spoil the accuracy. This can be achieved only if the inverse matrix possesses an approximation in the HKT format.

Approximability of the inverse matrix. Therefore, an important question to be asked prior to the computation of the inverse matrix is whether it holds true that A^{-1} can be approximated by a matrix in the $\mathrm{HKT}(\tilde r,\tilde s)$ format with some reasonably small $\tilde r$ and $\tilde s$ (prospectively, $\tilde r=\mathcal{O}(r)$ and $\tilde s=\mathcal{O}(s)$). In the case of $\mathcal{H}$-matrices such a question is answered in [2]. The approximability of the inverse in the HKT-format with the Kronecker rank $r=O(\log\varepsilon^{-1}\log\log\varepsilon^{-1})$, for a class of elliptic operators was proven in [11] (see also numerical experiments there).

Our numerical examples below show that in typical cases $\tilde r$ can be quite small.

Kronecker rank for A^{-1}	6	8	9	11	12	14
Relative error bound	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}

Table 2.1: Inverse Laplacian on a uniform rectangular grid

Example 1. Let A be the five-point stencil discretisation of the Laplacian on the uniform mesh on the unit rectangle in $\mathbb{R}^2$ (with the Dirichlet boundary conditions). It is easy to see that the Kronecker rank of A is 2. The approximate Kronecker ranks of A^{-1} for different values of relative approximation accuracy (in the Frobenius norm) are given in Table 2.1 ($n=64$ and, hence, $N=4096$). This indicates a logarithmic bound $\mathcal{O}(\log\varepsilon^{-1})$ for the approximate Kronecker rank.

Example 2. Let A be a function-value matrix for $f=1/|x-y|$ on a uniform mesh with respect to polar coordinates in the unit disc. The entries of the main diagonal of A are set to $2n$. Table 2.2 contains the approximate Kronecker ranks for A and A^{-1} ($n=64$, $N=4096$).

Kronecker rank for A	6	8	9	11	12	13
Kronecker rank for A^{-1}	10	12	14	16	18	20
Relative error bound	10^{-3}	10^{-4}	10^{-5}	10^{-6}	10^{-7}	10^{-8}

Table 2.2: Case of $1/|x-y|$ and polar coordinates in the unit disc

Numerical results on the accurate approximation of A^{-1} for the discrete finite difference Laplacian on the tensor-product grid $A \in \mathbb{R}^{N\times N}$, where $N = 1024^{256}$, are presented in [15].

3 Function Approximation by the Sinc Method

3.1 Sinc Approximation on a Rectangle

The given function $F(\zeta,\eta)$ is defined in the product domain $\Omega := (0,1)\times[a,b]$, $a,b\in\mathbb{R}$. We assume that for each fixed $\eta\in[a,b]$, the uni-variate function $F(\cdot,\eta)$ belongs to $C^\infty(0,1)$ and $F(0,\eta)=0$. Moreover, the function $F(\cdot,\eta)$ defined on $[0,1]$ is allowed to have singularity with respect to ζ at the end point $\zeta=0$ of $(0,1)$.

For this class of functions we construct a separable approximation of the form

$$F_r(\zeta,\eta)=\sum_{k=1}^{r}\Phi_k(\zeta)\Psi_k(\eta), \tag{3.1}$$

which will lead to the "almost exponential" decay

$$\|F-F_r\|_C \le \mathcal{O}(e^{-cr/\log r})$$

(cf. Theorem 3.1). Therefore the approximation accuracy $\varepsilon>0$ is achieved with $r(\varepsilon)=\mathcal{O}(|\log\varepsilon|\cdot\log|\log\varepsilon|)$ instead of $r(\varepsilon)=\mathcal{O}(|\log\varepsilon|)$ for "smooth" functions.

On the reference domain Ω, the function $F(\zeta,\eta)$ is analytic with respect to $\zeta\in(0,1)$, however, due to the singular behaviour at $\zeta=0$, one cannot expect an exponential convergence for the Taylor approximation or others polynomial interpolants. The idea is to use the so-called Sinc approximation (cf. [29]). This approach leads to a degenerate expansion (3.1) and was already successfully applied in [22] in the case of the so-called weak admissibility condition. In the following, we give a sketch of the corresponding results.

Through the transformation $z=\mathrm{Arcosh}(\frac{1}{x}) \leftrightarrow x=\frac{1}{\cosh(z)}$, where $\mathrm{Arcosh}(z):=\log(z+\sqrt{z^2-1})$, the approximation of the function $F(\zeta,\eta)$ is equivalent to the approximation of

$$g(z,\eta):=F\Big(\frac{1}{\cosh(z)},\eta\Big),\quad z\in\mathbb{R},\quad \eta\in[a,b]. \tag{3.2}$$

Let D_d^4 be the domain $D_d^4:=\left\{z=u+\mathrm{i}v : \frac{v^2}{\sin^2 d}-\frac{u^2}{\cos^2 d}\le 1\right\}$, where $0<d<\pi/2$ and let $D_d:=\{x+\mathrm{i}y : |y|<d\}$. Introduce the function $\phi(z)=\mathrm{Arsinh}\,z=\log(z+\sqrt{1+z^2})$ mapping D_d^4 conformally onto D_d. We define $H^1(D_d^4)$ as the family of all functions which are analytic in D_d^4 and such that $N(f\circ\psi,D_d)<\infty$ with $\psi(w)=\phi^{-1}(w)=\sinh(w)$, and

$$\int_{-d}^{d}|f(\psi(x+\mathrm{i}y))|dy\to 0\quad \text{as } x\to\pm\infty,$$

where

$$N(f,D_d)=\lim_{y\nearrow d}\left\{\int_{\mathbb{R}}|f(x+\mathrm{i}y)|\,dx+\int_{\mathbb{R}}|f(x-\mathrm{i}y)|\,dx\right\}.$$

Let

$$S_{k,\sigma}(x)=\frac{\sin[\pi(x-k\sigma)/\sigma]}{\pi(x-k\sigma)/\sigma} \tag{3.3}$$

be the kth Sinc function with step size $\sigma>0$, evaluated at $x\in\mathbb{R}$. The following theorem is based on the results in [26].

Theorem 3.1 *([22]) Let $g(z,\eta)$ be defined by (3.2). For any $\eta \in [a,b]$, assume $g(\cdot,\eta) \in H^1(D_d^4)$ with a norm $N(g(\cdot,\eta)\circ\psi, D_d) < \infty$ uniform in $\eta \in [a,b]$ and moreover, $|g(z,\eta)| \le ce^{-\alpha|z|}$, $z \in \mathbb{R}$, where α, c are positive constants. Choose $N \in \mathbb{N}$ and set $\sigma = (\log N)/N$. Then for any fixed $\eta \in [a,b]$, the* Sinc *interpolation using $z_k = 1/\cosh(\sinh(k\sigma))$ (note that $z_k = z_{-k}$) provides the error estimate*

$$\sup_{\zeta\in[0,1]} \left| F(\zeta,\eta) - \sum_{k=-N}^{N} F(z_k,\eta) S_{k,\sigma}\left(\phi\Big(\operatorname{Arcosh}(\frac{1}{\zeta})\Big)\right)\right| \le C\frac{N(g(\cdot,\eta)\circ\psi, D_d)}{d} e^{-\pi dN/\log N}. \tag{3.4}$$

Remark 3.2 *The separable ansatz*

$$F_r(\zeta,\eta) := \sum\nolimits_{m=-N}^{N} F(z_m,\eta) S_{m,\sigma}\left(\phi\Big(\operatorname{Arcosh}(\frac{1}{\zeta})\Big)\right) \equiv \sum\nolimits_{k=1}^{r} \Phi_k(\zeta)\Psi_k(\eta)$$

is a particular representation (3.1) with $\Phi_k(\zeta) = S_{k-1-N,\sigma}(\phi(\operatorname{Arcosh}(\frac{1}{\zeta})))$, $\Psi_k(\eta) = F(z_{k-1-N},\eta)$, leading to an explicit approximation to F with $r = N+1$ (due to $F(z_k,\eta) = F(-z_k,\eta)$).

3.2 Application to Standard Singularity Functions

In our context (see §2), we shall apply Theorem 3.1 to a function $F(\cdot,\cdot)$ associated with a primary kernel $f(x,y)$ generated by the fundamental solution of an elliptic operator with constant coefficients in $\mathbb{R}^d$, $d = 2, 3$. The function f is possibly modified according to §3.2.1.

In the following we use the common notation $x = (x_1, ..., x_d) \in \mathbb{R}^d$. Let $|x-y|$ denote the Euclidean distance in $\mathbb{R}^d$. In this section, we consider the following examples:
Example 1. $f(x,y) := \log|x-y|$, in Cartesian coordinates $x, y \in \mathbb{R}^2$.
Example 2. $f(x,y) := |x-y|^{-1}$, in Cartesian coordinates $x = (x_1, x_2, 0), y = (y_1, y_2, 0) \in \mathbb{R}^3$.
Example 3. $f(x,y) := \frac{e^{\mathrm{i}\kappa|x-y|}}{|x-y|}$, in Cartesian coordinates $x = (x_1, x_2, 0), y = (y_1, y_2, 0) \in \mathbb{R}^3$.

Further examples of the hierarchical Kronecker tensor-product approximation will be considered in Section 5.

3.2.1 Possible Modifications of the Function F

First, similarly to [22], we make the following remarks. If for each fixed $\eta \in [a,b]$ the function of interest $F(\zeta,\eta)$ is Hölder continuous in ζ at the end point $\zeta = 0$ of $[0,1]$, one can apply our approximation result to the modified function

$$\widetilde{F}(z,\eta) = F(z,\eta) - F(0,\eta), \tag{3.5}$$

which now satisfies the assumption $\widetilde{F}(0,\eta) = 0$. The second term in the right-hand side of (3.5) is already a separable function with $r = 1$.

If the target function $F(\zeta,\eta)$ has a stronger singularity at $\zeta = 0$ than allowed by Theorem 3.1, one can apply the above results to the following modified function

$$\widetilde{F}(z,\eta) = G(z,\eta) - G(0,\eta), \quad G(z,\eta) = \int_0^z F(u,\eta)du, \tag{3.6}$$

provided that the anti-derivative $G(z,\eta)$ is Hölder continuous at $z = 0$. This modification can be applied to the Galerkin discretisation in the case of piecewise linear basis functions after using partial integration (cf. [22]). Again, the second term in the right-hand side of (3.6) is already a separable function.

3.2.2 Example 1

Let $f(x,y) := \log|x-y|$, $x, y \in \mathbb{R}^2$. For $(\zeta,\eta) \in [0,1]\times[0,1]$, define the function

$$F(\zeta,\eta) := \log|x-y|, \qquad \zeta = |x_1 - y_1|, \quad \eta = |x_2 - y_2|,$$

which yields

$$F(\zeta,\eta) := \frac{1}{2}\log(\zeta^2 + \eta^2).$$

Now we introduce the function

$$F_0(\zeta,\eta) = \zeta^{\alpha_0} F(\zeta,\eta) \quad \text{with } 0 < \alpha_0 < 1,$$

corresponding to the choice (2.21) and $\mathcal{G}(\eta) = 1$ in (2.17). In the following, $h > 0$ denotes the maximal stepsize of the tensor-product grid.

Lemma 3.3 *For each $\varepsilon > 0$ there is an approximation to $F(\zeta,\eta)$ of the form*

$$F_r(\zeta,\eta) = \sum_{k=1}^{r} \frac{\Phi_{0k}(\zeta)}{\zeta^{\alpha_0}} \Psi_{0k}(\eta), \tag{3.7}$$

which leads to the following error bound for the corresponding Kronecker tensor-product approximation:

$$\|A - A_r\|_C \le C_1 \varepsilon, \tag{3.8}$$

where $C_1 = \mathcal{O}(h^4)$. The Kronecker rank of A_r is given by $r = \mathcal{O}(|\log\varepsilon| \cdot \log|\log\varepsilon|)$.

Proof. The function F_0 satisfies the assumptions of Theorem 3.1. Therefore, we obtain an approximation

$$\max_{\zeta,\eta} \left| F_0(\zeta,\eta) - \sum_{k=1}^{r} \Phi_{0k}(\zeta)\Psi_{0k}(\eta) \right| \le C e^{-cr/\log r} \le \varepsilon, \tag{3.9}$$

with Φ_{0k}, Ψ_{0k} defined in Remark 3.2 and $r := N + 1$. This leads to the desired separable approximation to F in the form $F_r = \zeta^{-\alpha_0} F_{0,r}(\zeta,\eta)$ which coincides with (3.7). Finally, we apply (2.20), where the condition $\alpha_0 < 1$ implies the uniform bound $C_1 = \mathcal{O}(h^4)$ for the involved integral. ∎

For our particular example, numerical results confirming an exponential convergence in (3.9) can be found in [22].

3.2.3 Example 2

Let $f(x,y) := |x-y|^{-1}$, $x, y \in \mathbb{R}^2$. For $(\zeta,\eta) \in [0,1] \times [0,b]$, define the function

$$F(\zeta,\eta) := |x-y|^{-1}, \qquad \zeta = |x_1 - y_1|, \quad \eta = |x_2 - y_2|,$$

yielding

$$F(\zeta,\eta) := \frac{1}{\sqrt{\zeta^2 + \eta^2}}.$$

Case A (Piecewise linear basis functions $\hat{\psi}^{i_1}$ with respect to x_1). We assume that the test functions satisfy the homogenous Dirichlet condition at the end points of the x_1-interval. For fixed $1 < \alpha_0 < 1$, introduce the function

$$G_0(\zeta,\eta) = \zeta^{\alpha_0} G(\zeta,\eta), \quad \text{where } G(\zeta,\eta) = \log(\zeta + \sqrt{\zeta^2 + \eta^2})$$

is the anti-derivative of F with respect to ζ.

Lemma 3.4 *For each $\varepsilon > 0$ there is an approximation*

$$\max_{\zeta,\eta} \left| G_0(\zeta,\eta) - \sum_{k=1}^{r} \Phi_{0k}(\zeta)\Psi_{0k}(\eta) \right| \le C e^{-cr/\log r} \le \varepsilon, \tag{3.10}$$

with Φ_{0k}, Ψ_{0k} defined in Remark 3.2. The corresponding degenerate approximation to $G(\zeta,\eta)$ takes the form

$$G_r(\zeta,\eta) = \sum_{k=1}^{r} \frac{\Phi_{0k}(\zeta)}{\zeta^{\alpha_0}} \Psi_{0k}(\eta), \tag{3.11}$$

which leads to the following error bound

$$\|A - A_r\|_C \le C_1 \varepsilon \tag{3.12}$$

with the Kronecker rank $r = \mathcal{O}(|\log\varepsilon| \cdot \log|\log\varepsilon|)$ and $C_1 = \mathcal{O}(h^4)$.

Proof. The function $G_0(\zeta,\eta)$ satisfies all assumptions in Theorem 3.1 with $0<\alpha<\alpha_0$. Therefore, again we obtain a separable approximation $G_{0,r}$ like in (3.9) with Φ_{0k}, Ψ_{0k} defined by (3.4). Here the error estimate (3.4) applies to the modified function $G_0(\zeta,\eta)$, which then yields (3.10). Now we construct a degenerate expansion for $G(\zeta,\eta)=\zeta^{-\alpha_0}G_0(\zeta,\eta)$ by means of

$$G_r(\zeta,\eta)=\zeta^{-\alpha_0}G_{0,r}(\zeta,\eta)$$

with $G_{0,r}$ described above, which then leads to (3.11). Clearly, (1.4) can be rewritten as

$$a_{i_1i_2j_1j_2}:=\iiiint F(|x_1-y_1|,|x_2-y_2|)\hat\phi^{i_1}(x_1)\hat\phi^{i_2}(x_2)\hat\phi^{j_1}(y_1)\hat\phi^{j_2}(y_2)dx_1dx_2dy_1dy_2. \tag{3.13}$$

Notice that integration by parts, (3.13) yields an equivalent representation

$$a_{i_1i_2j_1j_2}:=-\iiiint G(|x_1-y_1|,|x_2-y_2|)\left(\hat\phi^{i_1}(x_1)\right)'\hat\phi^{i_2}(x_2)\hat\phi^{j_1}(y_1)\hat\phi^{j_2}(y_2)dx_1dx_2dy_1dy_2,$$

which, in turn, results in the desired error bound (3.12) due to

$$\|A-A_r\|_C\le\varepsilon\max_{i_1,i_2,j_1,j_2}\iiiint\left|\frac{\left(\hat\phi^{i_1}(x_1)\right)'\hat\phi^{i_2}(x_2)\hat\phi^{j_1}(y_1)\hat\phi^{j_2}(y_2)}{|x_1-y_1|^{\alpha_0}}\right|dx_1dx_2dy_1dy_2 \tag{3.14}$$

with $\alpha_0<1$. ∎

Case B (Piecewise constant [or linear] basis functions with a mesh parameter $h>0$). We apply our approximation scheme on the domain $\Omega_\delta:=\Omega_1\cup\Omega_2$ with $\Omega_1:=[\delta,1]\times[0,\delta]$, $\Omega_2:=[0,1]\times[\delta,b]$, where $\delta\in(0,h]$ is small enough. On both Ω_1 and Ω_2, one can use a modification by (3.5). Furthermore, we define $F_r=0$ for $(\zeta,\eta)\in[0,\delta)\times[0,\delta)$, which introduces an error of the order $\mathcal{O}(\delta^\alpha)$ in the diagonal terms thanks to condition (3.19).

Finally, the constant $C=C(\delta)$ in (3.4) can be estimated by $\mathcal{O}(\delta^{-1})$, which leads to the bound

$$r=\mathcal{O}\left((|\log\delta|+|\log\varepsilon|)(\log|\log\delta|+\log|\log\varepsilon|)\right).$$

3.2.4 Example 3

On a 2D "screen" surface, we consider the singularity function corresponding to the 3D Helmholtz operator. Specifically, given $\kappa\in\mathbb{R}$, for $(x,y)\in[0,1]^2\times[0,b]^2$, in Cartesian coordinates $x=(x_1,x_2),y=(y_1,y_2)\in\mathbb{R}^2$, define the Helmholtz kernel function

$$f(x,y):=\frac{e^{\mathrm{i}\kappa|x-y|}}{|x-y|}.$$

It is worth noting that for $\kappa\neq0$ the Helmholtz kernel $f(x,y)$ does not belong to the class of asymptotically smooth functions. Therefore, the Taylor-based method in Section 4 cannot guarantee exponential convergence of a separable approximation. However, the Sinc method still provides an opportunity to construct a corresponding hierarchical tensor-product approximation. We mention that an analysis of polynomial approximations to the Helmholtz kernel function is presented in [20] in the context of the hierarchical matrix technique with standard admissibility criteria. Here we apply the corresponding Sinc approximation in the case of a weakly admissible block (cf. [22]) with respect to the transformed variables ζ,η.

We consider the case of piecewise constant basis functions. For $(\zeta,\eta)\in[0,1]\times[0,b]$, define

$$F(\zeta,\eta):=f(x,y),\qquad\zeta=|x_1-y_1|,\quad\eta=|x_2-y_2|,$$

which implies

$$F(\zeta,\eta):=\frac{e^{\mathrm{i}\kappa\sqrt{\zeta^2+\eta^2}}}{\sqrt{\zeta^2+\eta^2}}.$$

Similarly to Example 1, and using the representations (3.5), (2.17), we approximate the modified function

$$F_0(\zeta,\eta):=\zeta^{\alpha_0}(F(\zeta,\eta)-F(0,\eta)),\quad0<\alpha_0<1, \tag{3.15}$$

on the domain $\Omega_1:=[\delta,1]\times[0,b]$, where $\delta>0$ is a small parameter. The considerations for the remaining domain $\Omega_2:=[0,\delta]\times[\delta,b]$ are completely similar.

Lemma 3.5 *Given $r \in \mathbb{N}$, there is an approximation*

$$\max_{(\zeta,\eta)\in\Omega_1} \left| F_0(\zeta,\eta) - \sum_{k=1}^{r} \Phi_{0k}(\zeta)\Psi_{0k}(\eta) \right| \le C(\delta,\kappa) e^{-cr/\log r}, \tag{3.16}$$

where

$$C(\delta,\kappa) = \mathcal{O}(\delta^{-1} e^{\kappa b}). \tag{3.17}$$

Let $\delta = \mathcal{O}(\varepsilon^{1/4})$, then the corresponding Kronecker tensor-product approximation with the prescribed accuracy

$$\|A - A_r\|_C \le \varepsilon$$

has the Kronecker rank

$$r = \mathcal{O}((|\log\delta| + |\log\varepsilon| + \kappa)(\log|\log\delta| + \log|\log\varepsilon| + \log\kappa)). \tag{3.18}$$

Proof. The function F_0 satisfies the assumptions of Theorem 3.1 implying (3.16). In turn, the constant $C = C(\delta,\kappa)$ in (3.4) can be estimated by $\mathcal{O}(\delta^{-1}e^{\kappa b})$ (see [20] for more details). We use the analogous approximation on Ω_2 and then impose $F_r = 0$ on $[0,\delta)\times[0,\delta)$ which causes an error $\mathcal{O}(\delta^4)$. Now, substituting (3.17) into the required error estimate $C(\delta,\kappa)e^{-cN/\log N} \le \mathcal{O}(\varepsilon)$ leads to the bound (3.18). ∎

Clearly, for the large parameter κ the bound (3.18) does not provide a satisfactory complexity.

In our numerical tests below, we choose $\delta = 0.01$. However, corresponding to the theory, our numerics indicate that the approximation error depends only mildly on δ. For the function F_0 in (3.15) with $\kappa = 0.01, 1.0, 10$, $\eta = 0$, and for different values of r in (3.9), we obtain the following L_∞-norms of the error (cf. Fig. 3.1, with $r = M + 1$).

Figure 3.1: Error for the Sinc approximation to F_0 with $\kappa = 0.01, 1.0, 10$, respectively, from left to right.

Again, the above results clearly indicate an exponential convergence of the corresponding degenerate approximation. The pointwise error of the Sinc approximation to F_0 for $\kappa = 0.01$ and different r is depicted in Figure 3.2.

3.3 Kronecker Factors for the Sinc Method

Let us consider the Galerkin case (1.4) (the collocation case (1.5) is similar). As in Section 2, we require that the test functions possess the tensor-product form (2.13) and again, we use the same uni-variate functions in both dimensions.

In the following, we prove that the Kronecker factors U_k can be represented in the data-sparse format of hierarchical matrices while V_k allows a *global* low-rank approximation. The $\mathcal{H}$-matrix technique [16]-[23] (cf. also the mosaic-skeleton method [31, 32]) allows an efficient treatment of dense matrices arising from boundary element methods and the evaluation of volume integrals, etc. Moreover, the $\mathcal{H}$-format enables us to compute and store approximations to the inverses to finite element stiffness matrices in elliptic problems.

Figure 3.2: Pointwise error for the Sinc approximation to F_0 with $\kappa = 0.01$ for $r = 25$ (left), $r = 37$ (middle) and $r = 49$.

The hierarchical matrices are represented by means of a certain block partitioning. Figure 3.3 shows a typical block structure. Each block is filled by a submatrix of a rank not exceeding k. Then, for the mentioned class of matrices, it can be shown that the exact dense matrix $A \in \mathbb{R}^{n\times n}$ and the approximating hierarchical matrix $A_{\mathcal{H}}$ differ by $\|A - A_{\mathcal{H}}\| \le \mathcal{O}(\eta^k)$ for a certain number $\eta < 1$. This exponential decrease allows to obtain an error ε by the choice $k = \mathcal{O}(\log(1/\varepsilon))$. It is shown (e.g., in [17], [18], [19]) that the $\mathcal{H}$-matrix arithmetic exhibits the following complexity:

- *Data compression.* The storage of $n \times n$ $\mathcal{H}$-matrices as well as the matrix-vector multiplication and matrix-matrix addition have a cost of order $\mathcal{O}(kn \log n)$, where the local rank k is the parameter determining the approximation error.
- *Matrix-by-matrix and matrix-inverse complexity*[4]. The approximate matrix-matrix-multiplication and the inversion by truncation to the $\mathcal{H}$-matrix format take $\mathcal{O}\left(k^2 n \log^2 n\right)$ operations.

The $\mathcal{H}$-matrix approximations can be applied in the case of rather general triangulations (in particular, for locally refined grids). Since the case of non-uniform grids is technically more involved (see [21, 16] for more details), we assume quasi-uniformity.

Let the function F be defined on $\Omega = (0,1) \times [0,b]$. We consider the general case with the perturbed diagonal terms due to the construction $F_r = 0$ in $(\zeta,\eta) \in [0,\delta) \times [0,\delta)$ with $\delta \in (0,h]$ (see also Example 2 (case B)). We summarise the structural properties of U_k, V_k in the following theorem. Notice that in many particular cases the assumption (3.19) can be omitted (see Examples 1 - 3 from above).

Theorem 3.6 (shift-invariant functions) *Let A be a matrix of order $N = n^2$ defined by the Galerkin method with any quasi-uniform grid of the form (2.10), (2.11) with the minimal step size h. Let $\varepsilon = h^\alpha$, $\alpha > 0$, be a prescribed bound on the approximation error. Moreover, assume that a function F associated with $f(x,y)$ and modified by (3.5), satisfies the assumptions of Theorem 3.1 and let F satisfy the condition*

$$\sup_{x_1,y_1} \iint\limits_{|x_2-y_2|\le\delta} |F(x_1-y_1, x_2-y_2)|dx_2dy_2 = \mathcal{O}(\delta^\alpha) \qquad \text{as } \delta \to 0. \tag{3.19}$$

Then A can be approximated by a matrix A_r in the Kronecker tensor-product format (1.3) so that the entry-wise accuracy is $\mathcal{O}(\varepsilon)$, where $r = \mathcal{O}(\log\varepsilon^{-1} \cdot \log\log\varepsilon^{-1})$.

Furthermore, let also $\widetilde{F} = F(z_k,\eta) - F(z_k,0)$ satisfy the assumptions of Theorem 3.1, but now with respect to η uniformly for all $z_k \in [0,1]$. Then we obtain low-rank Kronecker factors V_k and $\mathcal{H}$-matrices U_k (both with rank $k = \mathcal{O}(\log\varepsilon^{-1})$) so that the storage for A_r is $\mathcal{O}(rn\log n\log\varepsilon^{-1})$ and the matrix-by-vector complexity for A_r is $\mathcal{O}(rn^2\log n\log\varepsilon^{-1})$. Similar results hold for approximations applied to F_0 in (2.17).

[4]The term *matrix-by-matrix complexity* is an abbreviation for the complexity of the matrix-matrix multiplication. The *matrix-inverse complexity* is the complexity of the matrix inversion.

Proof. We apply the most general construction in §3.2.3 (cf. Example 2, Case B) to the modified function in (3.5). Due to Theorem 3.1 and Remark 3.2 this leads to the separable approximation of $F(\zeta,\eta)$, $\zeta=(x_1-y_1)^2$, $\eta=(x_2-y_2)^2$, in the form (2.9) with $r=\mathcal{O}(\log\varepsilon^{-1}\cdot\log\log\varepsilon^{-1})$.

Clearly, both U_k and V_k are nothing but the Galerkin stiffness matrices for the integral operators generated by the kernel functions $\Psi_k(x_2,y_2)$ and $\Phi_k(x_1,y_1)$ defined in general on the intervals $[0,1]$, $[0,b]$ and by the Galerkin basis $\{\hat\phi^i(x_2)\}$ and $\{\hat\phi^i(x_1)\}$, respectively (cf. (2.13)). In fact, the matrix entries of the Kronecker factors $U_k=\{u_k(i_2,j_2)\}$ and $V_k=\{v_k(i_1,j_1)\}$ with $1\le i_1,j_1,i_2,j_2\le n$, are given by

$$u_k(i_2,j_2)=\iint\Psi_k(x_2,y_2)\hat\phi^{i_2}(x_2)\hat\phi^{j_2}(y_2)dx_2dy_2,\quad v_k(i_1,j_1)=\iint\Phi_k(x_1,y_1)\hat\phi^{i_1}(x_1)\hat\phi^{j_1}(y_1)dx_1dy_1.$$

The approximability of U_k and V_k by hierarchical matrices now relies on the separability properties of the kernel functions $\Psi_k(x_2,y_2)$ and $\Phi_k(x_1,y_1)$.

Due to Remark 3.2, we find that $\Phi_k(x_1,y_1):=S_{k-1-N,\sigma}(\phi(\mathrm{Arcosh}(1/\zeta)))$ with $\zeta=(x_1-y_1)^2$ is generated by the kth Sinc function (cf. (3.3)) which is smooth (analytic) in ϕ and thus in ζ except the point $\zeta=0$. Given the constant $p\in\mathbb{N}$, $p\ge 2$. Then on the interval $[ph,1]$, the function $S_{k-1-N,\sigma}(\phi(\mathrm{Arcosh}(1/\zeta)))$ can be approximated by piecewise polynomials of the total degree $s=\mathcal{O}(\log\varepsilon^{-1}\cdot\log\log\varepsilon^{-1})$ with the accuracy $\varepsilon=h^\alpha$. In fact, it is easy to check that the function $S_{k-1-N,\sigma}(\phi(\mathrm{Arcosh}(1/\zeta)))$ (cf. (3.3)) has at most $O(\log\log h^{-1})$ zeroes on the interval $\zeta\in[ph,1]$. Moreover, on each interval between two neighbouring zeroes it can be approximated by a polynomial of degree $\mathcal{O}(\log\varepsilon^{-1})$. Therefore, the Galerkin matrix V_k can be approximated by a diagonal plus a (global) rank-s matrix $\tilde V_k$ with the entry-wise accuracy $\varepsilon>0$, where $s=\mathcal{O}(\log\varepsilon^{-1}\cdot\log\log\varepsilon^{-1})$.

On the other hand, we have $\Psi_k(x_2,y_2):=F(z_k,\eta)$, where $F(z_k,\eta)$ might be singular at $\eta=0$. Due to the assumption on $F(z_k,\cdot)$, we can apply the $\mathcal{H}$-matrix format based on both the standard and weak admissibility condition (cf. [22]) to approximate the corresponding Galerkin matrix U_k with the local rank $s=\mathcal{O}(\log\varepsilon^{-1})$. This proves the assertion. ∎

Remark 3.7 *Assume that the $\mathcal{H}^2$-matrix format (cf. [23, 4]) is applicable to represent the matrices U_k, $V_k\in\mathbb{R}^{n\times n}$, $n=\sqrt{N}$. Then the overall storage and matrix-by-vector complexity will be reduced to $\mathcal{O}(rn\log\varepsilon^{-1})$ and $\mathcal{O}(rn^2\log\varepsilon^{-1})$, respectively.*

Notice that for fixed ε, the complexity of the matrix-vector-multiplication by the Kronecker factors U_k and V_k is linear in n.

3.4 Recompression by the *SVD*-Method

Despite the constructive proof of Theorem 3.6 (cf. also Theorem 4.5), it may serve rather like an "existence theorem" leaving room for other possible approximation algorithms to run in practice. Even if A_r is determined strictly in the lines of that proof, there may be unnecessarily many Kronecker-product terms, i.e., the construction from above is not claimed to be optimal.

Once some A_r has been found, we can try to approximate it by another matrix with fewer Kronecker-product terms. Due to Remark 2.1, this reduces to looking for a *lower-rank* approximation to a given *low-rank* matrix. The latter task is called *recompression* (cf. [33], [4]) and can be done very efficiently by standard algebraic tools as follows. Note that the following algorithm uses the Frobenius Norm $\|\cdot\|_F$ instead of $\|\cdot\|_C$.

Algorithm 3.8 *Given $U,V\in\mathbb{C}^{n\times r}$ and a prescribed recompression accuracy $\varepsilon>0$, the aim is to find $\hat U,\hat V\in\mathbb{C}^{n\times\hat r}$ with $\hat r\le r$ and $\|\hat U\hat V^\top-UV^\top\|_F\le\varepsilon\|UV^\top\|_F$.*

1. *Compute the QR decomposition for U and V:*

$$U=Q_UR_U,\quad V=Q_VR_V,\qquad Q_U,Q_V\in\mathbb{C}^{n\times r},\quad R_U,R_V\in\mathbb{C}^{r\times r},$$

   where Q_U, Q_V have orthonormal columns and R_U, R_V are upper triangular.

2. *Compute the singular value decomposition for $M=R_UR_V^\top$:*

$$M=\mathbb{U}\begin{bmatrix}\sigma_1&&\\&\ddots&\\&&\sigma_r\end{bmatrix}\mathbb{V}^T,$$

where $\sigma_1 \geq \ldots \geq \sigma_r$ are the singular values of M and $\mathbb{U}, \mathbb{V} \in \mathbb{C}^{r\times r}$ are unitary matrices.

3. *Find the minimal $\hat{r}$ such that*

$$\sqrt{\sigma_{\hat{r}+1}^2 + \ldots + \sigma_r^2} \leq \varepsilon \sqrt{\sigma_1^2 + \ldots + \sigma_r^2}.$$

4. *Denote by $\mathbb{U}_{\hat{r}}$ and $\mathbb{V}_{\hat{r}}$ the first $\hat{r}$ columns in $\mathbb{U}$ and $\mathbb{V}$, respectively, and set*

$$\hat{U} = Q_U \mathbb{U}_{\hat{r}} \begin{bmatrix} \sigma_1 & & \\ & \ddots & \\ & & \sigma_{\hat{r}} \end{bmatrix}, \qquad \hat{V} = Q_V \mathbb{V}_{\hat{r}}.$$

After the recompression by Algorithm 3.8, the columns of $\hat{U}$ and $\hat{V}$ become approximations to the singular vectors of the original matrix (up to scaling in the case of $\hat{U}$).

Our numerical experiments definitely point to the hierarchical structure of these matrices, strikingly, this is the $\mathcal{H}$-matrix structure.

For example, take the Cartesian product of two identical uniform grids on $[0, 1]$ with n nodes and consider the case

$$a(i, j) = a(i_1, i_2; j_1, j_2) = F(\zeta_{i_1,j_1}, \eta_{i_2,j_2}), \quad i \leftrightarrow (i_1, i_2),\ j \leftrightarrow (j_1, j_2) \tag{3.20}$$

with

$$F(\zeta, \eta) = 1/\sqrt{\zeta^2 + \eta^2}.$$

In this particular case, $n = 256$ and $N = n^2 = 65\,536$ is chosen. The recompression procedure (having started with $r = 10$) yields $\hat{r} = 9$ Kronecker-product terms with the relative approximation accuracy $7.7{\cdot}10^{-4}$ (in the Frobenius norm). The construction of the initial Kronecker tensor-product approximation was performed via the incomplete cross approximation procedure from [33] (cf. also [7]) and took 1.2 seconds (on a Pentium-1600 notebook), while the recompression by Algorithm 3.8 took 0.8 seconds.

Using the columns of $\hat{U}$ and $\hat{V}$, we construct the Kronecker factors $U_1, \ldots, U_{\hat{r}}$ and $V_1, \ldots, V_{\hat{r}}$. All these Kronecker factors manifest a similar structure. In particular, the U_1 and V_1 Kronecker factors (stemming from the singular vectors for the largest singular value) show a simple hierarchical structure (see Figure 3.3).

Figure 3.3: $\mathcal{H}$-matrix structure of the singular-vector Kronecker factors.

The rank of non-diagonal blocks in Figure 3.3 happens to be ≤ 4; the $\mathcal{H}$-matrix storage is about 19% of the initial storage for the same Kronecker factor (which is quite satisfactory for a matrix of order $n = 256$). The computation was performed by the algorithm from [31] (the construction applies an idea similar to those used in adaptive quadrature rules).

We conjecture that the $\mathcal{H}$-matrix structure in the singular-vector Kronecker factors is not occasional. However, up to now the proof open. Maybe it needs a better insight into the properties of the singular functions of the operators related to our matrices.

It was already mentioned that the structure of $\hat{A}$ is similar to that arising in the $\mathcal{H}$-matrix technique via weak admissibility. The corresponding generalisation of adaptive cross approximation (cf. [22]) can be also applied to construct the initial Kronecker tensor-product approximation (see [22] for numerical examples

for the case $F(\zeta,\eta)=\log(\zeta+\eta)$). Therefore, the same $\mathcal{H}$-matrix structure can also directly (i.e., without recompression) arise for the hierarchical piecewise polynomial interpolation after modifications according to [22, Subsection 3.2.2] or for the Sinc-based method (see §3.1).

4 Function Approximation by Piecewise Polynomial Expansions

4.1 Approximation Error

Now we start our analysis in the case of asymptotically smooth functions (resulting in Theorems 4.5 and 4.6). As it is found at the end of Section 2, the problem essentially reduces to the study of function approximations to F of low separation rank.

Consider first the function-value case (1.6) and assume shift-invariance (2.7), (2.8) with

$$0 \le x_1, x_2, y_1, y_2 \le 1$$

and, hence,

$$-1 \le \zeta, \eta \le 1.$$

Following [34], let us assume that $F(\zeta,\eta)$ is *asymptotically smooth* in the sense that there exist constants $g\in\mathbb{R}$ and $c,t>0$ such that

$$\left|\frac{\partial^{p_1+p_2}}{(\partial\zeta)^{p_1}\,(\partial\eta)^{p_2}}\,F(\zeta,\eta)\right| \;\le\; c\,t^{p_1+p_2}\,(p_1+p_2)!\,(\zeta^2+\eta^2)^{(g-p_1-p_2)/2} \tag{4.1}$$

for any integers $p_1,p_2\ge p_0\ge 0$ (with a given constant p_0) and all $(\zeta,\eta)\in[-1,1]^2\setminus\{(0,0)\}$. Note that F might be singular at the origin $\zeta=\eta=0$, which is the midpoint of $[-1,1]^2$.

Consider $\Pi_\delta=[-1,1]^2\setminus(-\delta,\delta)^2$ for some $\delta>0$. As proved in [34], Π_δ can be represented as a union of disjoint rectangles D_ν, $1\le\nu\le\mu$ (the explicit description will follow):

$$\Pi_\delta=\bigcup_{1\le\nu\le\mu} D_\nu, \tag{4.2}$$

so that F has a uniform (piecewise) separable approximation on each D_ν, i.e., there are separable approximations $F_{\nu,p}$ on D_ν containing p terms and leading to an uniform accuracy $\mathcal{O}(\gamma^p)$ on D_ν for some $\gamma\in(0,1)$. Extending the functions $F_{\nu,p}$ by zero outside of D_ν, we obtain $\bar F_{\nu,p}$ defined on Π_δ. The agglomerated sum $\sum_\nu \bar F_{\nu,p}$ is a uniform separable approximation of F on the whole of Π_δ with $p\mu$ terms.

More precisely, the family of these rectangles has a hierarchical structure. First, Π_δ is covered by inflating "rectangular rings" as follows:

$$\Pi_\delta \;\subset\; \bigcup_k \mathcal{R}(a_k), \qquad \mathcal{R}(a_k)=[-(s+1)a_k,\;(s+1)a_k]^2\setminus(-sa_k,\;sa_k)^2,$$
$$a_k=\left(1+\tfrac{1}{s}\right)^k\;\tfrac{h}{s},\quad k=0,1,\dots,$$

where s is any fixed number such that $s>t$ (t from (4.1)) and is used then to set $\gamma:=t/s$. Second, $\mathcal{R}(a_k)$ consists of the four rectangles

$$\begin{array}{ll}
[-(s+1)a_k,-sa_k]\times[(-(s+1)+\alpha)a_k,(-s+\alpha)a_k], & \alpha=0,1,\dots,2s,\\
[sa_k,(s+1)a_k]\times[(-(s+1)+\alpha)a_k,(-s+\alpha)a_k], & \alpha=0,1,\dots,2s,\\
[(-(s+1)+\beta)a_k,(-s+\beta)a_k]\times[-(s+1)a_k,-sa_k], & \beta=1,2,\dots,2s-1,\\
[(-(s+1)+\beta)a_k,(-s+\beta)a_k]\times[sa_k,(s+1)a_k], & \beta=1,2,\dots,2s-1,
\end{array}$$

and the D_ν from (4.2) are all rectangles of this form (in some ordering) involved to cover Π_δ. For later references, we abbreviate the boundary points of D_ν by

$$D_\nu=[\zeta_1^\nu,\zeta_2^\nu]\times[\eta_1^\nu,\eta_2^\nu]. \tag{4.3}$$

As is readily seen, $\mu=\mathcal{O}(\log\delta^{-1})$ with δ from the definition of Π_δ.

Consider any of the D_ν with centre $(\zeta_{\nu,0}, \eta_{\nu,0})$ and approximate $F(\zeta,\nu)$ on D_ν by the Taylor expansion

$$F_{\nu,p}(\zeta,\eta) = \sum_{\ell=0}^{p-1} \frac{1}{\ell!} \left((\zeta-\zeta_{\nu,0})\ \frac{\partial}{\partial\xi_1} + (\eta-\eta_{\nu,0})\ \frac{\partial}{\partial\xi_2} \right)^{\ell} F(\xi_1,\xi_2) \Bigg|_{\xi_1=\zeta_{\nu,0},\ \xi_2=\eta_{\nu,0}}. \tag{4.4}$$

Collecting the terms with equal monomials, we come up with p separable terms as follows:

$$F_{\nu,p}(\zeta,\eta) = \sum_{\ell=0}^{p-1} c_{\nu,\ell} (\zeta-\zeta_{\nu,0})^{\ell} (\eta-\eta_{\nu,0})^{p-\ell}. \tag{4.5}$$

Also, due to (4.1), we obtain the following error estimate (cf. [34]):

$$|F(\zeta,\eta) - F_{\nu,p}(\zeta,\eta)| \ \le\ \text{const}\cdot\ \gamma^p\ (\zeta^2+\eta^2)^{g/2} \qquad \text{for all } (\zeta,\eta)\in D_\nu. \tag{4.6}$$

Let $F_r(\zeta,\eta)$ be obtained by agglomeration of the $F_{\nu,p}$ functions. If $\varepsilon \sim \gamma^p$ and $\delta \sim \varepsilon^\alpha$ for some $\alpha > 0$, then

$$r = \mathcal{O}(\log^2 \varepsilon^{-1}), \quad \max_{\zeta,\eta\in\Pi_\delta} \left| \frac{F(\zeta,\eta) - F_r(\zeta,\eta)}{(\zeta^2+\eta^2)^{g/2}} \right| = \mathcal{O}(\varepsilon). \tag{4.7}$$

Now we apply the above function approximation results to build up the Kronecker tensor-product approximations of the function-value matrix (1.6). Given a grid $x^i \in [0,1]^2$ of the form (2.10), set

$$\zeta_{i_1 j_1} = x_1^{i_1} - x_1^{j_1}, \qquad \eta_{i_2 j_2} = x_2^{i_2} - x_2^{j_2} \tag{4.8}$$

and suppose that (3.20) holds.

Denote by h the minimal step-size of the one-dimensional grids. Then, evidently, $(\zeta_{i_1,j_1}, \eta_{i_2,j_2}) \in \Pi_h$ whenever $i \ne j$. Let A_r be defined by (2.5), (2.12). Then its main diagonal turns out to be zero. The diagonal entries $a(i,i)$ of A form the diagonal matrix D. Hence, we arrive at the approximation $A_{r,D} := D + A_r$ of the form (1.2).

While D is the diagonal of A, $\tilde{D} = \mathcal{P}(D)$ is a certain part of the rearranged matrix $\tilde{A} = \mathcal{P}(A)$ (see Section 2). Note that $\tilde{D}$ is not the diagonal of $\tilde{A}$ as illustrated below for the case $n = 3$:

$$D = \left[\begin{array}{ccc|ccc|ccc} d_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & d_2 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & d_3 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & d_4 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & d_5 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & d_6 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & d_7 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & d_8 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & d_9 \end{array}\right], \quad \mathcal{P}(D) = \left[\begin{array}{ccc|ccc|ccc} d_1 & 0 & 0 & 0 & d_4 & 0 & 0 & 0 & d_7 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ d_2 & 0 & 0 & 0 & d_5 & 0 & 0 & 0 & d_8 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ \hline 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ d_3 & 0 & 0 & 0 & d_6 & 0 & 0 & 0 & d_9 \end{array}\right].$$

Under the present assumptions, D is a scalar matrix (i.e., a multiple of the identity). Hence, $\mathcal{P}(D)$ is of rank 1 and D is exactly the Kronecker product of two $n\times n$ matrices adding a $(r+1)$st term to A_r. Thus, the format (1.2) is not needed, since $A_{r,D} = D + A_r = A_{r+1}$.

We may take $\delta > h$. This will lead to a band of zeros in the A_r and the format (1.2) with D being now a band-like matrix.

Quite the opposite, for the collocation and Galerkin cases, we may take a sufficiently small δ (see last paragraph of Section 2). If $\delta \sim \varepsilon^\alpha$ for some $\alpha > 0$ (and hence not extremely small) we are eventually led to the conclusion that $r = \mathcal{O}(\log^2 \varepsilon^{-1})$.

4.2 Kronecker Factors in the Case of Piecewise Polynomial Approximation

In the previous section, we have already built a bridge from function approximations (of low separation rank) to matrix approximations (of low Kronecker rank) assuming the function-value case (1.6) and the grid condition (2.10). Now we are in the position to analyse the structure of the corresponding Kronecker factors.

Consider definition (3.20). Then the Taylor-based construction of Section 4 yields Kronecker factors U_k and V_k that are associated with the rectangles D_ν, except for possibly one pair allied with the main diagonal. More precisely, p pairs U_k, V_k are related to one D_ν. Let $U_{k+\ell}$, $V_{k+\ell}$, $0 \le \ell \le p-1$, be the factors associated with a fixed ν. Due to (4.5), neglecting the coefficients $c_{\nu,\ell}$, we obtain

$$\begin{array}{lll} u_{k+\ell}(i_2, j_2) = (x_2^{i_2} - x_2^{j_2} - \eta_{\nu,0})^{p-\ell}, & \eta_1^\nu \le x_2^{i_2} - x_2^{j_2} \le \eta_2^\nu, & 1 \le i_2, j_2 \le n, \\ v_{k+\ell}(i_1, j_1) = (x_1^{i_1} - x_1^{j_1} - \zeta_{\nu,0})^{\ell}, & \zeta_1^\nu \le x_1^{i_1} - x_1^{j_1} \le \zeta_2^\nu, & 1 \le i_1, j_1 \le n, \end{array} \tag{4.9}$$

where the values on the left side hold only for indices satisfying the inequality restrictions; otherwise, $u_{k+\ell}(i_2, j_2) = v_{k+\ell}(i_1, j_1) = 0$.

There are two important observations on the matrices $U_{k+\ell}$ and $V_{k+\ell}$. First, due to the imposed limitations on the indices, we recognise a band structure (in the case of uniform grids) or a more general pattern which we call a *profile* pattern (see the definition below). (We remark that the band width or the number of entries inside the profile pattern will not be important for us, the only essential property is the shape of the pattern.) Second, if there were no limitations on the indices, the $U_{k+\ell}$ and $V_{k+\ell}$ would be low-rank matrices, of rank $p-\ell+1$ and $\ell+1$, respectively. The combination of the profile-pattern and low-rank properties can be defined rigorously as follows.

Definition 4.1 *Let $G = [g_{\alpha\beta}]_{1 \le \alpha, \beta \le n}$ be an $n \times n$-matrix, and assume that there are indices*

$$\tau_1 \le \tau_2 \le \ldots \le \tau_n, \qquad \tau_1' \le \tau_2' \le \ldots \le \tau_n', \qquad \tau_1 \le \tau_1', \ldots, \tau_n \le \tau_n', \tag{4.10}$$

such that $g_{\alpha\beta} = 0$ whenever $\beta \notin [\tau_\alpha, \tau_\alpha']$. Furthermore, assume that there is a matrix $\tilde{G}$ with $\operatorname{rank} \tilde{G} \le p$ and coinciding with G at all entries (α, β) subject to $\beta \in [\tau_\alpha, \tau_\alpha']$. Then G is said to be a profile-rank-p matrix or - in the case of $p \ll n$ - a profile-low-rank matrix.

The $\tau_\alpha, \tau_\alpha'$ indices describe the "support" (i.e., the non-zero part) of G, while the (usually dense) matrix $\tilde{G}$ can be viewed as extension satisfying the rank restriction. Vice versa, G can be considered as the restriction of some rank-p matrix $\tilde{G}$ to the support defined by (4.10). As discussed above, the extensions $\tilde{U}_{k+\ell}$, $\tilde{V}_{k+\ell}$ of the matrices $U_{k+\ell}$, $V_{k+\ell}$ from (4.9) are defined by the left side in (4.9) for all indices.

Clearly, a profile-rank-p matrix is completely determined by the $\tau_\alpha, \tau_\alpha'$ indices and the vectors u_k, v_k of a rank-p decomposition

$$\tilde{G} = \sum_{k=1}^{p} u_k v_k^\top, \quad u_k, v_k \in \mathbb{C}^n,$$

of $\tilde{G}$. Thus, the storage reduces to $\mathcal{O}(pn)$ (instead of n^2 for a dense $n \times n$ matrix).

Remarkably, the same reduction can be achieved for the matrix-by-vector complexity if the following algorithm is applied. Here, the components of u_k and v_k are denoted by $u_{\alpha,k}$ and $v_{\beta,k}$, respectively.

Algorithm 4.2 *Given $x = [x_\beta]_{1 \le \beta \le n}$, compute $y = [y_\alpha]_{1 \le \alpha \le n} := Gx$ as follows:*

1. *Compute*

$$s_{1,k} = \sum_{\beta=\tau_1}^{\tau_1'} v_{\beta,k} x_\beta \qquad \text{for all } 1 \le k \le p.$$

2. *For $\alpha = 2, \ldots, n$ compute*

$$s_{\alpha,k} = s_{\alpha-1,k} + \sum_{\beta=\tau_{\alpha-1}'+1}^{\tau_\alpha'} v_{\beta,k} x_\beta - \sum_{\beta=\tau_{\alpha-1}}^{\tau_\alpha - 1} v_{\beta,k} x_\beta \qquad \text{for all } 1 \le k \le p.$$

3. *For $\alpha = 1, \ldots, n$ compute*

$$y_\alpha = \sum_{k=1}^{p} u_{\alpha,k} s_{\alpha,k} \qquad \text{for all } 1 \le k \le p.$$

It is easy to see that the number of arithmetic operations in Algorithm 4.2 does not exceed

$$2p\left(n+\tau_1'-\tau+1+\sum_{\alpha=2}^{n}(\tau_\alpha'-\tau_{\alpha-1}')+\sum_{\alpha=2}^{n}(\tau_\alpha-\tau_{\alpha-1})\right) \;=\; \mathcal{O}(pn).$$

Proposition 4.3 *Let A_r be a matrix of order $N=n^2$ of the form (1.3) and its Kronecker factors be profile-rank-p matrices of order n. Then, using the Kronecker tensor-product format and exploiting the band-low-rank structure of the factors, the storage for A_r is $\mathcal{O}(rp\sqrt{N})$ and the matrix-by-vector complexity is $\mathcal{O}(rpN)$.*

For the proof, it will suffice to recall the general scheme delivering $y=(U\times V)x$. Using (2.2)-(2.4), we write

$$a(i,j)=a(i_1,i_2;j_1,j_2)=u(i_2,j_2)v(i_1,j_1),$$
$$y(i)=y(i_1,i_2),\quad x(j)=x(j_1,j_2),\qquad i\leftrightarrow(i_1,i_2),\quad j\leftrightarrow(j_1,j_2),$$

for the components of A,U,V and x,y. Then,

$$y(i_1,i_2)=\sum_{j_1=1}^{n}\sum_{j_2=1}^{n}u(i_2,j_2)v(i_1,j_1)x(j_1,j_2). \tag{4.11}$$

This can be accomplished by the following steps.

Algorithm 4.4 *Given $U,V\in\mathbb{C}^{n\times n}$ and $x\in\mathbb{C}^N$, $N=n^2$, the aim is to determine $y=(U\times V)x$. For the start, consider x as an $n\times n$ matrix $X=[x(j_1,j_2)]$.*

1. *Compute $Z=[z(i_1,j_2)]=VX$.*
2. *Compute $W=[w(i_2,i_1)]=UZ^\top$.*
3. *Set $Y=[y(i_1,i_2)]=W^\top$.*

The target vector y comes up free as the vectorised form of Y.

Thus, the multiplication of one Kronecker-product matrix by a vector reduces to two standard matrix-matrix products and two transpositions. The corresponding complexity is dominated by the costs to compute VX and $UZ^\top$.

Since the multiplication of two matrices can be reduced to the matrix-vector multiplication of the first matrix by the columns of the second, the profile-low-rank structure in U and V can be used straightforwardly.

Altogether, what we have found in the analysis of approximate matrix structures under the Taylor-based approach can be summarised in the following theorem.

Theorem 4.5 *Let A be a matrix of order $N=n^2$ defined by (3.20) with an arbitrary asymptotically smooth function F and any grid of the form (2.10), (2.11) with the minimal step-size h of the involved one-dimensional grids. Let $\varepsilon=h^\alpha$, $\alpha>0$, be a prescribed bound on the approximation error.*

Then A can be approximated by a matrix A_r in the Kronecker tensor-product format (1.3) with the profile-low-rank Kronecker factors so that $r=\mathcal{O}(\log^2\varepsilon^{-1})$ and the entrywise accuracy is $\mathcal{O}(\varepsilon)$, while the storage for A_r is $\mathcal{O}(rn\log^3\varepsilon^{-1})$ and the matrix-by-vector complexity for A_r is $\mathcal{O}(rn^2\log^3\varepsilon^{-1})$.

Note that the proposed new format definitely outperforms the format of m-term Kronecker products (related to multi-way algorithms from [25]) by a factor of order $N^{1/m}$ (see Introduction) both concerning storage and matrix-by-vector complexity.

It seems pertinent to remark that the profile-low-rank format can be viewed as a particular case of the $\mathcal{H}$-format with the blocks refined actually towards some "profile lines" in the matrix. In this case, the hierarchical structure of blocks arises due to a certain piecewise smoothness of the function generating the entries. Note that a similar case was considered in [31] (the paper presents the concept of "mosaic rank" and a purely algebraic proof for a piecewise constant structure of an $n\times n$ matrix to result in an $\mathcal{O}(n\log n)$ storage and the same matrix-by-vector complexity).

Similar theorems can be obtained as well for the collocation and Galerkin cases.

Theorem 4.6 *Let A be a matrix of order $N = n^2$ defined by (1.5) or (1.4) with a shift-invariant f expressed by (2.7) through an arbitrary asymptotically smooth function F. Assume that the test functions are of the tensor-product form (2.13), where the uni-variate test functions are ordered according to (2.16). In the collocation case, the grid is assumed to satisfy (2.10) and (2.11). Assume that there exists $\alpha > 0$ such that (3.19) holds. Then A can be approximated by a matrix A_r in the Kronecker tensor-product format (1.3) with profile-low-rank Kronecker factors so that $r = \mathcal{O}(\log^2 \varepsilon^{-1})$ and the entrywise accuracy is $\mathcal{O}(\varepsilon)$, while the storage for A_r is $\mathcal{O}(rn \log^3 \varepsilon^{-1})$ and the matrix-by-vector complexity for A_r is $\mathcal{O}(rn^2 \log^3 \varepsilon^{-1})$.*

Proof. Choose δ so that $\varepsilon = \delta^\alpha$. Due to (3.19), the integration over the regions intersecting with $|x_1 - x_2| \le \delta$ or $|y_1 - y_2| \le \delta$ contributes to the entries (1.5) or (1.4) and their approximations (2.14) or (2.15) by an order of $\mathcal{O}(\varepsilon)$. Thus, we obtain the same $\mathcal{O}(\log^2 \varepsilon^{-1})$ bound on r. Note that the domain $(-\delta, \delta)^2$ close to the singularity is excluded from the set Π_δ, where the separable approximations are determined with accuracy $\mathcal{O}(\varepsilon)$. ∎

5 Approximation of Non-Shift-Invariant Kernels

The hierarchical Kronecker tensor-product approximation is not restricted to the class of shift-invariant kernel functions. Below we extend our approach to polar and spherical coordinates, where the distance function $|x - y|$ is no longer shift-invariant.

5.1 Approximation in Polar Coordinates

Consider the 2D volume potential $f(x, y) := \log |x - y|$ in polar coordinates $x = (\rho_x, \theta_x)$, $y = (\rho_y, \theta_y) \in \mathbb{R}^2$, where $x_1 = \rho_x \cos\theta_x$, $x_2 = \rho_x \sin\theta_x$, $y_1 = \rho_y \cos\theta_y$, $y_2 = \rho_y \sin\theta_y$. Using the representation

$$|x - y| = \sqrt{(\rho_x - \rho_y)^2 + 4\rho_x\rho_y \sin^2 \frac{1}{2}(\theta_x - \theta_y)}\,, \tag{5.1}$$

we rewrite the kernel function in the form

$$\log |x - y| = \frac{1}{2} \log \rho_x\rho_y + \frac{1}{2} \log \left(\frac{(\rho_x - \rho_y)^2}{\rho_x\rho_y} + 4 \sin^2 \frac{\theta_x - \theta_y}{2} \right).$$

Since the first term in the right-hand side is already separable, we concentrate on the second term which we name again by F:

$$F(\zeta, \eta) := \log \left(\frac{(\rho_x - \rho_y)^2}{\rho_x\rho_y} + 4 \sin^2 \frac{\theta_x - \theta_y}{2} \right), \qquad \eta = \frac{|\rho_x - \rho_y|}{\sqrt{\rho_x\rho_y}}, \quad \zeta = 2|\sin \frac{\theta_x - \theta_y}{2}|.$$

Using the variables ζ, η, there holds

$$F(\zeta, \eta) := \log \left(\zeta^2 + \eta^2\right), \qquad (\zeta, \eta) \in [0, 2] \times [0, \infty).$$

Again introducing the function

$$F_0(\zeta, \eta) = \zeta^{\alpha_0} (F(\zeta, \eta) - F(b, \eta)) \qquad \text{with } 0 < \alpha_0 < 1,$$

we apply the Sinc approximation with respect to ζ as in Example 1 (cf. §3.2.1) and obtain

$$F_{0,r}(\zeta, \eta) = \sum_{k=1}^{r} \Phi_{0k}(\zeta) \Psi_{0k}(\eta), \qquad r = N + 1, \tag{5.2}$$

with Φ_{0k}, Ψ_{0k} defined by (3.4). The analysis of a separable approximation

$$F_r = \zeta^{-\alpha_0} F_{0,r} + F(b, \eta)$$

with $F_{0,r}$ in (5.2) (which generates the Kronecker tensor-product approximation of the corresponding Galerkin stiffness matrix) is almost the same as in Example 1. However, there are two issues requiring special considerations:

- more careful analysis of the Kronecker factors since now the function $F(\zeta_k, \eta)$, $\eta \in [0, \infty)$, may have singularities not only on the manifold $\rho_x - \rho_y = 0$, but also at $\rho_x = 0$ and $\rho_y = 0$;
- the unbounded domain of F with respect to η so that $|F(\cdot, \eta)| \to \infty$ as $\eta \to \infty$.

The first item will be discussed in §5.4. Concerning the second item, we note that there holds

$$|F(\zeta, \eta) - F(b, \eta)| \le C < \infty$$

uniformly in $(\zeta, \eta) \in [0, b] \times [0, \infty)$. Therefore, the constant C in (3.4) is uniformly bounded and we arrive essentially at the same approximation result for F_r as in Example 1.

5.2 Approximation on Surfaces

Consider the single layer potential $f(x, y) := |x - y|^{-1}$, $x, y \in \Gamma$, where Γ is a rotational surface in $\mathbb{R}^3$ generated by a Hölder continuous function $h(\rho)$, $\rho \in [0, b]$, with $h(0) = h(b) = 0$. In this case we have $x = (\rho_x, h(\rho_x), \theta_x)$, $y = (\rho_y, h(\rho_y), \theta_y) \in \mathbb{R}^3$, such that

$$|x - y| = \sqrt{(h(\rho_x) - h(\rho_y))^2 + (\rho_x - \rho_y)^2 + 4h(\rho_x)h(\rho_y)\sin^2\frac{1}{2}(\theta_x - \theta_y)}\,. \tag{5.3}$$

First, we represent the target kernel function in the form

$$|x - y|^{-1} = \frac{1}{\sqrt{h(\rho_x)h(\rho_y)}} \frac{1}{\sqrt{\frac{(h(\rho_x)-h(\rho_y))^2+(\rho_x-\rho_y)^2}{h(\rho_x)h(\rho_y)} + 4\sin^2\frac{1}{2}(\theta_x - \theta_y)}} \tag{5.4}$$

and then consider the modified function F corresponding to the second factor in the right-hand side above

$$F(\zeta, \eta) := \frac{1}{\sqrt{\zeta^2 + \eta^2}}, \quad \zeta^2 := 4\sin^2\frac{\theta_x - \theta_y}{2}, \quad \eta^2 := \frac{(h(\rho_x) - h(\rho_y))^2 + (\rho_x - \rho_y)^2}{h(\rho_x)h(\rho_y)} \tag{5.5}$$

in the domain $(\zeta, \eta) \in \Omega := [0, 2] \times [0, \infty)$.

In the case of piecewise linear basis functions in θ, the further construction will be similar to that in Example 2 except the two issues already mentioned in Section 5.1. Thus we obtain a separable approximation F_r to F.

Besides one has to take into account that the corresponding error $||A - A_r||_C$ includes the integration over a surface with the weight function $(h(\rho_x)h(\rho_y))^{1/2}$ since $dxdy = h(\rho_x)h(\rho_y)d\theta_x d\rho_x d\theta_y d\rho_y$. Finally, we have

$$\begin{aligned}\|A - A_r\|_C &\le \max_{i_1,i_2,j_1,j_2} \iiiint \sqrt{h(\rho_x)h(\rho_y)}\left|(F - F_r)\hat\phi^{i_1}(\theta_x)\hat\phi^{i_2}(\theta_y)\hat\phi^{j_1}(\rho_x)\hat\phi^{j_2}(\rho_y)\right| d\theta_x d\rho_x d\theta_y d\rho_y \qquad (5.6)\\ &\le \varepsilon \max_{i_1,i_2,j_1,j_2} \iiiint \sqrt{h(\rho_x)h(\rho_y)}\left|\frac{\left(\hat\phi^{i_1}(\theta_x)\right)'\hat\phi^{i_2}(\theta_y)\hat\phi^{j_1}(\rho_x)\hat\phi^{j_2}(\rho_y)}{|\theta_x - \theta_y|^{\alpha_0}}\right| d\theta_x d\rho_x d\theta_y d\rho_y\end{aligned}$$

with $\alpha_0 < 1$.

5.3 Separable Change of Variables

There is the following general observation allowing to get rid of the shift-invariance requirement of f. As previously, let

$$f(x_1, x_2, y_1, y_2) = F(\zeta, \eta), \tag{5.7}$$

but now suppose that

$$\begin{aligned}\zeta(x_1, y_1, x_2, y_2) &= \sum_{l=1}^{r_1} S_l^1(x_1, y_1)S_l^2(x_2, y_2),\\ \eta(x_1, y_1, x_2, y_2) &= \sum_{l=1}^{r_2} T_l^1(x_1, y_1)T_l^2(x_2, y_2).\end{aligned} \tag{5.8}$$

Assume that all functions involved are bounded. Hence, if $0 \le x_1, x_2, y_1, y_2 \le 1$, then ζ and η belong to a finite interval, say, $[a, b]$.

Let F be an arbitrary, asymptotically smooth function. Then, by the Taylor-based constructions of Section 4, we approximate F on $[a, b]^2 \backslash [-\delta, \delta]^2$ for some small δ by F_r, where F_r is the sum of r terms, each being a polynomial in ζ times a polynomial in η. Substituting ζ and η by their expressions (5.8) and using the polynomial representation of F_r, we obtain separable approximations with the same estimate on r as we have had in the shift-invariant case. Due to Remark 2.1 and 2.2, we arrive at approximations A_r of A with the Kronecker rank r.

For a further analysis of the structure of the Kronecker factors, we need some additional assumptions. Let us also require that

$$\begin{array}{ll} S_l^1(x_1, y_1) = S^{1x}(x_1) S_l^{1y}(y_1), & S_l^2(x_2, y_2) = S^{2x}(x_2) S_l^{2y}(y_2), \\ T_l^1(x_1, y_1) = T^{1x}(x_1) T_l^{1y}(y_1), & T_l^2(x_2, y_2) = T^{2x}(x_2) T_l^{2y}(y_2). \end{array} \tag{5.9}$$

Substituting (5.9) into the polynomials of the separable expansion of F_r, we discover that the Kronecker factors are restrictions of low-rank matrices to a certain non-zero pattern (the rank depends on r and also on r_1 and r_2).

This general observation helps, for instance, when we work in the *polar coordinates*. In this case we set

$$\begin{array}{ll} x_1 = \rho_x \cos\theta_x, & x_2 = \rho_x \sin\theta_x, \\ y_1 = \rho_y \cos\theta_y, & y_2 = \rho_y \sin\theta_y, \end{array} \tag{5.10}$$

and then obtain

$$\begin{array}{rcccl} \zeta(\rho_x, \rho_y, \theta_x, \theta_y) & = & x_1 - y_1 & = & \rho_x \cos\theta_x - \rho_y \cos\theta_y, \\ \eta(\rho_x, \rho_y, \theta_x, \theta_y) & = & x_2 - y_2 & = & \rho_x \sin\theta_x - \rho_y \sin\theta_y. \end{array} \tag{5.11}$$

Obviously, we enjoy (5.8) and (5.9) simultaneously. Consequently, the hierarchical (piecewise low-rank) Kronecker tensor-product approximations are taken for granted in the polar coordinates under the same assumptions on the grids and test functions as were considered earlier in the Cartesian coordinates.

5.4 Kronecker Factors in the Case of Non-Shift-Invariant Functions

In the non-shift-invariant case (cf. §5), the analysis of structures and complexities of the Kronecker factors can be slightly different from those in the shift-invariant case because of the following issues:

(i) The function $\Psi_k(\eta)$ (related to $F(\zeta_k, \eta)$, $\eta \in [0, \infty)$) may have singularities not only on the manifold $\rho_x - \rho_y = 0$, but also at $\rho_x = 0$ and $\rho_y = 0$ (see §§5.1-5.2);

(ii) usually, we have an unbounded domain of F with respect to η, $(\zeta, \eta) \in [0, b] \times [0, \infty)$;

(iii) the error bound $\|A - A_r\|_C$ may include an integration with a singular weight function in ρ_x, ρ_y (cf. (5.6));

(iv) the lack of Toeplitz or circulant structure even for uniform meshes.

First, consider the case of §5.1. Using the representation

$$F(z_k, \eta) = \log\left((\rho_x - \rho_y)^2 + \rho_x \rho_y z_k\right) - \log\left(\rho_x \rho_y\right)$$

with $\eta = \eta(\rho_x, \rho_y)$ according to (5.5), we see that the second term is already separable, while the first one is unbounded only at the diagonal $\rho_x = \rho_y$. (If $\rho_x = \rho_y$, the term $\log(\rho_x \rho_y z_k)$ tends to infinity as $z_k \to 0$). Therefore the standard $\mathcal{H}$-matrix structure provides a good approximation to U_k. Again, all matrices V_k allow a global low-rank approximation. Concerning item (ii), we have already mentioned that the "shifted" function $F(\zeta, \eta) - F(b, \eta)$ remains regular as $\eta \to \infty$.

Topic (iii) arises within the error estimate (5.6). Since all singularities in (5.6) are absolutely integrable, the corresponding integral has the bound $\mathcal{O}(h^4)$ as in the shift-invariant case. Furthermore, we use the representation

$$F(z_k, \eta) = \frac{\sqrt{h(\rho_x) h(\rho_y)}}{\sqrt{(h(\rho_x) - h(\rho_y))^2 + (\rho_x - \rho_y)^2 + h(\rho_x) h(\rho_y) z_k}},$$

where the numerator is already a separable function but the denominator leads to singularities only at $\rho_x = \rho_y \in \{0, b\}$, while F becomes unbounded if $\rho_x = \rho_y$ and $z_k \to 0$.

Altogether, we obtain the same structure of the Kronecker factors as in the shift-invariant case. Finally, we remark that the lack of Toeplitz/circulant structures in the variables ρ_x, ρ_y is irrelevant for our approach.

6 Conclusion and Conjectures

The main result of this paper is Theorem 3.6 (cf. also Theorems 4.5, 4.6). The first one assumes that the function used in the generation of the matrices admits some analytical properties with certain behaviour at the singularity point in the origin while the second and third ones assume asymptotical smoothness of this function. Theorem 3.6 covers all typical singularity functions in the method of integral equations (however, we do not prove that asymptotically smooth functions are included in the set of analytic functions under consideration). In particular, Theorem 3.6 establishes existence of the Kronecker tensor-product approximations (with Kronecker rank $r = \log \varepsilon^{-1} \cdot \log\log \varepsilon^{-1}$) wich allows the $\mathcal{H}$-matrix structure in the Kronecker factors, with an $\mathcal{O}(n \log n \log \varepsilon^{-1})$ storage and $\mathcal{O}(n^2 \log n \log \varepsilon^{-1})$ matrix-by-vector complexity up to the factor $\log\log \varepsilon^{-1}$.

The "existence theorems" in this paper are proved constructively by the following two methods:

(a) global Sinc approximations (Theorem 3.6)

(b) hierarchical piecewise polynomial approximations (Theorems 4.5, 4.6).

However, a practically useful option can be an algebraic method as discussed in Section 3.4, with the recompression procedure reducing the Kronecker rank of a preliminary Kronecker tensor-product approximation obtained by any available method (say, mentioned in topics (a), (b) above).

We conjecture that after the recompression the Kronecker factors are well-approximated by $\mathcal{H}$-matrices. It is confirmed by numerical experiments, but the proof would need a better insight into the properties of the singular vectors of the involved matrices and related operators.

Several conjectures and lines for future research are raised in Section 2.2. The following questions will be addressed in the forthcoming papers:

- The existence of approximate, specially structured vectors in practical problems (leading to a sub-linear matrix-by-vector complexity). The possibility to keep the special structure of the vectors in computational processes such as PCG or GMRES.
- The possibility of truncation of the Kronecker rank in matrix-by-matrix operations.
- Fast approximate algorithms for computation of the inverse matrices in the HKT format in the cases which are not covered by [11].

We also believe that the HKT format may be useful in problems involving multiplications of integral operators and matrix resolvents (in particular, to represent general matrix-valued functions, cf. [3, 8, 9, 10]). It might also lead to new fast approximate algorithms for matrix transforms on irregular grids.

A challenging question pertains to the possibility of weakening our assumptions on the grids and test functions (see the discussion at the end of the Introduction). We envisage that the HKT format can be beneficially coupled with certain interpolation approaches.

Finally, we stress that our HKT approximations can be successfully applied in the case $d > 2$ providing feasible operator calculus in higher dimensions (cf. [11], [15]).

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