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Boris N. Khoromskij

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Tensor-structured Preconditioners and Approximate Inverse of Elliptic Operators in $\mathbb{R}^d$

Boris N. Khoromskij
Max-Planck-Institute for Mathematics in the Sciences,
Inselstr. 22-26, D-04103 Leipzig, Germany.
{bokh}@mis.mpg.de

Dedicated to Prof. I. Gavrilyuk on the occasion of his 60-th birthday.

Abstract

In the present paper we analyse a class of tensor-structured preconditioners for the multidimensional second order elliptic operators in $\mathbb{R}^d$, $d \geq 2$. For equations in bounded domain the construction is based on the rank-R tensor-product approximation of the elliptic resolvent $\mathcal{B}_R \approx (\mathcal{L} - \lambda I)^{-1}$, where $\mathcal{L}$ is the sum of univariate elliptic operators. We prove the explicit estimate on the tensor rank R that ensures the spectral equivalence. For equations in unbounded domain one can utilise the tensor-structured approximation of Green's kernel for the shifted Laplacian in $\mathbb{R}^d$, that is well developed in the case of non-oscillatory potentials. For the oscillating kernels $\frac{e^{-i\kappa\|x\|}}{\|x\|}$, $x \in \mathbb{R}^d$, $\kappa \in \mathbb{R}_+$ we constructive proof of the rank-$O(\kappa)$ separable approximation. This leads to the tensor representation for the discretized 3D Helmholtz kernel on $n \times n \times n$ grid that requires only $O(\kappa\,|\log\varepsilon|^2\, n)$ reals for storage. Such representations can be applied to both the 3D volume and boundary calculations with sublinear cost $O(n^2)$ even in the case $\kappa = O(n)$.

Numerical illustrations demonstrate the efficiency of low tensor rank approximation for Green's kernels $\frac{e^{-\lambda\|x\|}}{\|x\|}$, $x \in \mathbb{R}^3$, in the case of Newton ($\lambda = 0$), Yukawa ($\lambda \in \mathbb{R}_+$) and Helmholtz ($\lambda = i\kappa$, $\kappa \in \mathbb{R}_+$) potentials, as well as for the kernel functions $1/\|x\|$ and $1/\|x\|^{d-2}$, $x \in \mathbb{R}^d$, in higher dimensions $d > 3$. We present numerical results on the iterative calculation of the minimal eigenvalue for the d-dimensional finite difference Laplacian by power method with the rank truncation and based on the approximate inverse $\mathcal{B}_R \approx (-\Delta)^{-1}$, with $3 \leq d \leq 50$.

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1 Introduction

The construction of efficient preconditioned iterative methods plays the important role in the numerical analysis of high dimensional equations arising in the modern engineering, physical and chemistry applications. For example, we mention the multi-dimensional integral-differential equations, elliptic/parabolic boundary value problems posed in $\mathbb{R}^d$, $d \geq 2$,

which include the Hartree-Fock/Kohn-Sham equations in density functional theory, the time-dependent Schrödinger equation in quantum molecular dynamics, the Lippmann-Schwinger integral formulation of the electronic Schrödinger and Hartree-Fock equations, the Poisson-Boltzmann equation in protein modelling, the deterministic Boltzmann equation as well as the multi-parametric stochastic PDEs.

In multi-dimensional applications, traditional numerical methods of linear complexity in the volume fail due to the so-called "curse of dimensionality" (Bellman). This effect can be relaxed or completely avoided by a systematic application of low rank tensor-structured representations of the arising multivariate functions and related operators. Applications of tensor methods for representation of classical Green's kernels and elliptic resolvent [3, 4, 11, 13, 19, 23, 2], multi-dimensional convolution [21, 20, 6] and many other quantities arising in electronic structure calculations [17, 22, 24] have demonstrated the surprising efficiency. In some applications the a-priori fixed tensor subspace via sparse grids leads to efficient algorithms in higher dimensions [12, 31].

The present paper is motivated by the fact that application of tensor formats for iterative solving of the elliptic boundary-value and spectral problems in higher dimensions is essentially based on using preconditioned (nonlinear) iterations with tensor truncation (cf. [3, 4, 16, 20, 14, 26]). In this way the construction of spectrally close tensor structured preconditioners for the class of elliptic integral-differential operators in $\mathbb{R}^d$ is one of the building blocks in development of efficient numerical methods in the case $d \geq 3$.

The idea on tensor-structured approximation of the elliptic inverse was first addressed in [3, 4]. Particular constructions based on the sinc-approximation applied to the operators $(-\Delta+\lambda I)^{-\alpha}$, $\lambda \in \mathbb{R}_+$, $\alpha > 0$ on a hypercube were considered in [11, 20]. In the present paper we prove the explicit estimate on the tensor rank of sinc-quadrature based preconditioners that ensures spectral equivalence. Efficient tensor approximation of non-oscillatory free-space Green's kernels for different discretisation schemes have been described [17, 13, 19]. To our best knowledge, the low rank tensor-structured approximation for oscillating kernels have not been yet addressed in the literature (cf. the asymptotically optimal method in the volume size based on the fast multipole type representations [5, 6]). In the present paper we construct and prove the rank-$O(\kappa)$ separable approximation for the oscillating kernel $\frac{e^{-i\kappa\|x\|}}{\|x\|}$, $x \in \mathbb{R}^d$, $\kappa \in \mathbb{R}_+$. Such representations allow the 3D volume and boundary calculations with sublinear cost $O(|\log\varepsilon|\,\kappa n)$, even in the case $\kappa = O(n)$. Notice that methods presented in [5, 6] lead to the linear complexity in the volume, $O(\kappa^3 \log\kappa + C(|\log\varepsilon|)^3)$.

The rest of the paper is organised as follows. In Section 2 we formulate the classes of boundary-value and spectral problems in bounded/unbounded domains and formulate the tensor truncated preconditioned iterative schemes. We also collect some basic definitions on the separable approximation of multivariate functions (tensors) and related operators (matrices). Then we introduce the class of tensor structured preconditioners for elliptic operators of the second order. We also discuss possible applications of the separable approximation for the free-space Green's kernels in the so-called FEM-BEM coupling methods and in the Green function formulations. In Section 3, we analyse the tensor-product preconditioner in $(0,1)^d$. Lemma 3.1 shows the linear scaling in d, while Lemma 3.2 proves the explicit estimate on the tensor rank that ensures spectral equivalence. Then, we focus on tensor-product approximation of the integral operators in $\mathbb{R}^d$ with oscillating kernels. We give constructive proof of the rank-$O(\kappa)$ separable approximation for the oscillating kernel function $\frac{e^{-i\kappa\|x\|}}{\|x\|}$,

$x \in \mathbb{R}^d$, $\kappa \in \mathbb{R}_+$. This leads to the tensor representation with approximation error $\varepsilon > 0$, for the discretized 3D Helmholtz fundamental solution on $n \times n \times n$ grid that requires only $O(|\log \varepsilon|^2 n^2)$ reals for storage.

We complete Section 3 with report on the results of numerical experiments illustrating the efficiency of the low tensor-rank approximation for the class of nonoscillating kernels for $d \geq 3$, and for the oscillating Helmholtz kernel in 3D. Another numerical example shows the linear scaling in d of the "truncated" power iteration (cf. [14]) applied to the spectral problem for the Laplacian in $(0,1)^d$, $d \leq 50$.

2 Problem setting and description of preconditioners

2.1 Problem setting

We consider preconditioning methods for solving boundary value and eigenvalue problems

$$\Lambda u = f, \quad \text{and} \quad \Lambda u = \lambda u \tag{2.1}$$

with the elliptic differential operator Λ of the form

$$\Lambda := -\operatorname{div}(A\nabla u) + Vu. \tag{2.2}$$

Here the operator Λ maps as $\Lambda : H_0^1(\Omega) \to H^{-1}(\Omega)$, where $\Omega \subset \mathbb{R}^d$ is some bounded or unbounded tensor-product domain. The operator coefficients $A = \{a_{ij}(x)\}_{i,j=1}^d \in C^\infty(\Omega, \mathbb{R}^{d\times d})$, and $V \in C(\Omega)$ in (2.2) are supposed to provide the low tensor-rank approximation of the corresponding solutions in $H_0^1(\Omega)$ (see [14, 26]).

Efficient numerical solvers for high-dimensional boundary value and eigenvalue problems can be based on systematic use of the tensor approximation methods (cf. [3, 4, 11, 15, 13]). This concept relies on several prerequisites:

- Representation of arising operators and functions in rank-structured tensor formats and the corresponding error analysis (separable approximation).
- Efficient implementation of multilinear matrix-vector operations with truncation to fixed tensor rank (tensor truncation).
- Construction of rank-structured spectrally close preconditioners or approximate inverse operators and using them in special iterative solvers which are well suited for truncated iterations.

The last topic will be in the focus of the present paper.

2.2 Tensor-structured representation of functions and operators

In this section we recall the commonly used tensor structured formats for representing the high order tensors considered as the elements of tensor-product Hilbert space [29].

Representation of tensors: A d-th order tensor $V = [v_{i_1,\ldots,i_d} : i_\ell \in I_\ell] \in \mathbb{R}^{\mathcal{I}}$ ($\mathcal{I} = I_1 \times \ldots \times I_d$) is an element of the tensor-product Hilbert space $\mathbb{V}_{\mathbf{n}} = \otimes_{\ell=1}^d \mathbb{V}_\ell$ of real-valued

(complex-valued) functions of the discrete argument, with $\mathbb{V}_\ell = \mathbb{R}^{I_\ell}$, and equipped with the Euclidean *inner product* $\langle\cdot,\cdot\rangle : \mathbb{V}_{\mathbf{n}} \times \mathbb{V}_{\mathbf{n}} \to \mathbb{R}$, where $\mathbf{n} = (n_1, ..., n_d)$. In general, we have $I_\ell = \{1, ..., n_\ell\}$, however, for the ease of discussion we set $\#I_\ell = n_\ell = n$ $(\ell = 1, ..., d)$. The concept of rank-structured tensor product formats allows to get rid of the exponential increase in the number of entries in V, as n^d. In this way, one considers the *outer product* of vectors $v^{(\ell)} = \{v^{(\ell)}_{i_\ell}\}_{i_\ell \in I_\ell} \in \mathbb{V}_\ell$ $(\ell = 1, ..., d)$ that forms the canonical rank-1 tensor

$$V \equiv [v_{\mathbf{i}}]_{\mathbf{i}\in\mathcal{I}} = v^{(1)} \otimes ... \otimes v^{(d)} \in \mathbb{V}_{\mathbf{n}} \quad \text{with entries} \quad v_{\mathbf{i}} = v^{(1)}_{i_1} \cdots v^{(d)}_{i_d},$$

requiring only dn elements to store it (now linear in the dimension). In the case $d = 2$, the outer product of vectors represents a rank-1 matrix.

Rank-R canonical representation (tensor class $\boldsymbol{\mathcal{C}}_{R,\mathbf{n}}$) of a tensor $V \in \mathbb{V}_{\mathbf{n}}$ is defined by

$$V = \sum\nolimits_{\nu=1}^{R} \beta_\nu v^{(1)}_\nu \otimes \ldots \otimes v^{(d)}_\nu, \quad \beta_\nu \in \mathbb{R} \tag{2.3}$$

with normalised vectors $v^{(\ell)}_\nu \in \mathbb{V}_\ell$ $(\ell = 1, ..., d)$. The minimal parameter R in (2.3) is called the rank (or canonical rank) of a tensor.

Tucker model (tensor class $\boldsymbol{\mathcal{T}}_{\mathbf{r},\mathbf{n}}$, $\mathbf{r} = (r_1, ..., r_d)$): Rank-$\mathbf{r}$ orthogonal Tucker approximation is based on subspaces $\mathbb{T}_{\mathbf{n}} := \otimes_{\ell=1}^{d} \mathbb{T}_\ell \subset \mathbb{V}_{\mathbf{n}}$ for certain $\mathbb{T}_\ell = span\{t^{(\ell)}_{\nu_\ell}\}_{\nu_\ell=1}^{r_\ell} \subset \mathbb{V}_\ell$ with $r_\ell := \dim \mathbb{T}_\ell < n$. Then each tensor $V \in \mathbb{T}_{\mathbf{n}}$ can be represented by a sum of rank-1 elements

$$V = \sum\nolimits_{\nu_1=1}^{r_1} \ldots \sum\nolimits_{\nu_d=1}^{r_d} \beta_{\nu_1,\ldots,\nu_d}\, t^{(1)}_{\nu_1} \otimes \ldots \otimes t^{(d)}_{\nu_d} \equiv \boldsymbol{\beta} \times_1 T^{(1)} \times_2 T^{(2)} ... \times_d T^{(d)}, \tag{2.4}$$

where $T^{(\ell)} = [t^{(\ell)}_1 ... t^{(\ell)}_{r_\ell}]$, $t^{(\ell)}_{\nu_\ell} \in \mathbb{T}_\ell$ $(\ell = 1, ..., d)$ is the orthogonal matrix and $\times_\ell$ denotes the mode-ℓ contracted product. Here $r = \max\limits_{\ell}\{r_\ell\}$ is called the Tucker rank ($Trank$). In our applications we have $r \ll n$, say $r = O(\log n)$. The coefficients tensor $\boldsymbol{\beta} = [\beta_{\nu_1,\ldots,\nu_d}] \in \mathbb{R}^{r_1\times\ldots\times r_d}$ (core tensor), is an element of the dual (reciprocal) tensor space $\mathbb{B}_{\mathbf{r}}$.

Remark 2.1 *Note that $\mathcal{C}_R$ is a subset of $\mathcal{T}_{\mathbf{r}}$ with $\mathbf{r} = (R, ..., R)$ corresponding to the case of diagonal core tensors. Hence, we have the following lower bound on the canonical rank in (2.3), in terms of the Tucker rank in (2.4), $r = \max_\ell r_\ell \le R$.*

Mixed (two-level) Tucker-canonical model: Subclass $\boldsymbol{\mathcal{T}}_{\mathcal{C}_{R,\mathbf{r}}} \subset \boldsymbol{\mathcal{T}}_{\mathbf{r},\mathbf{n}}$ with $\boldsymbol{\beta} \in \boldsymbol{\mathcal{C}}_{R,\mathbf{r}} \subset \mathbb{B}_{\mathbf{r}}$, consists of tensors in the form

$$V = \Big(\sum\nolimits_{\nu=1}^{R} \beta_\nu b^{(1)}_\nu \otimes \ldots \otimes u^{(d)}_\nu\Big) \times_1 T^{(1)} \times_2 T^{(2)} ... \times_d T^{(d)}, \tag{2.5}$$

where $T^{(\ell)} \in \mathbb{R}^{n\times r_\ell}$ $(\ell = 1, ..., d)$ is the orthogonal matrix.

Storage constraints: The storage requirements for the Tucker (resp. canonical) decomposition is bounded by $r^d + drn$ (resp. $R + dRn$), where usually $r \ll n$ and $r \ll R$. Representing the $\boldsymbol{\mathcal{T}}_{\mathcal{C}_{R,\mathbf{r}}}$ format amounts to $dRr + R + drn$ reals (linear scaling in d, n, R, r).

Representation of tensor-structured matrices (operators): The index sets $I_1, ..., I_d$ and $J_1, ..., J_d$ give rise to the pair of tensor-product Hilbert spaces $V = \mathbb{R}^{I_1} \otimes ... \otimes \mathbb{R}^{I_d}$ and $W = \mathbb{R}^{J_1} \otimes ... \otimes \mathbb{R}^{J_d}$. Given matrices $A^{(\ell)} \in \mathbb{R}^{I_\ell \times J_\ell}$ $(\ell = 1, ..., d)$, their Kronecker product $\mathcal{A} := A^{(1)} \otimes ... \otimes A^{(d)}$ is defined as the mapping

$$\mathcal{A} : V \to W, \quad V \ni v = v^{(1)} \otimes ... \otimes v^{(d)} \mapsto \mathcal{A}v = A^{(1)}v^{(1)} \otimes ... \otimes A^{(d)}v^{(d)} \in W.$$

We introduce a class $\boldsymbol{\mathcal{M}}_{R,\mathbf{n}}$ of the Kronecker rank R ($Krank(\mathcal{A}) = R$) matrices in the form

$$\mathcal{A} = \sum\nolimits_{\nu=1}^{R} A_\nu^{(1)} \otimes \cdots \otimes A_\nu^{(d)}, \quad A_\nu^{(\ell)} \in \mathbb{R}^{I_\ell \times J_\ell}, \quad \ell = 1, ..., d, \tag{2.6}$$

where R is supposed to be small, say $R = O(\log n)$. This provides a *tremendous reduction in storage* from $\mathcal{O}(n^{2d})$ to $\mathcal{O}(dRn^2)$. The matrices $A_\nu^{(\ell)}$ can be "compressed" by techniques of hierarchical or wavelet matrix approximation or adapting Toeplitz/circulant type structures (cf. the convolution with translation invariant kernels) reducing the complexity and storage to $\mathcal{O}(dRn \log n)$.

Low tensor rank nonlinear approximation: Since both $\boldsymbol{\mathcal{T}}_{\mathbf{r}}$ and $\boldsymbol{\mathcal{C}}_R$ are not linear spaces, we arrive at a nontrivial nonlinear approximation problem

$$A_0 \in \mathbb{V}_{\mathbf{n}}: \quad A = \mathrm{argmin}_{T \in \mathcal{S}} \|A_0 - T\|_{\mathbb{V}_{\mathbf{n}}} \tag{2.7}$$

with $\mathcal{S} \in \{\boldsymbol{\mathcal{T}}_{\mathbf{r}}, \boldsymbol{\mathcal{C}}_R, \boldsymbol{\mathcal{T}}_{\mathcal{C}_{R,\mathbf{r}}}\}$ or $\mathcal{S} \subset \boldsymbol{\mathcal{T}}_{\mathbf{r}}$ being a subclass of symmetric, antisymmetric, or positive tensors. The replacement of A_0 by an approximation $A \in \mathcal{S}$ is called the *tensor truncation* to $\mathcal{S}$ and denoted by $T_{\mathcal{S}} A_0$. In practice, the computation of the minimiser A can be performed only approximately.

In the case $\mathcal{S} = \boldsymbol{\mathcal{T}}_{\mathbf{r}}$, we have proven the solvability of minimisation problem (2.7), the quadratic convergence in the "energy functional", and analysed the structure of its Frechét derivative (cf. [19]). Basic ALS iteration to compute the Tucker approximation in $\boldsymbol{\mathcal{T}}_{\mathbf{r}}$ was presented in [7, 8]. With good initial guess, we normally observe the stable geometric convergence of the ALS method for *orthogonal* Tucker approximation. On the other hand, the (nonorthogonal) canonical decomposition in $\boldsymbol{\mathcal{C}}_R$ is well suited for fast multilinear algebra. The mixed tensor format $\boldsymbol{\mathcal{T}}_{\mathcal{C}_{R,\mathbf{r}}}$ combined with the multigrid acceleration techniques allows to utilise the favourable features of both Tucker and canonical models [24].

2.3 Equations in bounded domain

We are interested in preconditioned iterations for solving the FEM approximations of the variational boundary-value problem

$$\text{find } u \in H_0^1(\Omega) \text{ s.t.} \quad \int_\Omega \sum_{i,j=1}^{d} a_{ij}(x) \partial_i u \partial_j v + V u v = \int_\Omega f v \qquad \forall v \in H_0^1(\Omega), \tag{2.8}$$

as well as of the related eigen-value problem: Find $(\lambda, u) \in \mathbb{R} \times H_0^1(\Omega) \setminus \{0\}$, such that

$$\int_\Omega \sum_{i,j=1}^{d} a_{ij}(x) \partial_i u \partial_j v + V u v = \lambda \int_\Omega u v \qquad \forall v \in H_0^1(\Omega). \tag{2.9}$$

For numerical approximation and preconditioning of "tensor-structured" discrete elliptic operators defined in the hypercube $\Omega = (0,1)^d$, we consider the Galerkin schemes via the tensor-product piecewise polynomial basis functions $\{\phi_{\mathbf{i}}\}$,

$$\phi_{\mathbf{i}}(x) = \prod_{\ell=1}^{d} \phi_{i_\ell}(x_\ell), \quad \mathbf{i} \in \mathcal{I} = I^d := \{1, ..., n\}^d. \tag{2.10}$$

For the ease of presentation, ϕ_{i_ℓ} are supposed to be linear polynomials in variable x_ℓ, i.e., we choose the Galerkin subspace of the Courant hat functions, $\mathbb{V}_n = (V_n)^d \subset (H_0^1(0,1))^d$ associated with the uniform tensor product grid. The Galerkin approximation to the initial BVP (2.8) now reads as follows

$$\mathcal{L}U \equiv (\mathcal{A}+\mathcal{V})U = F, \quad U \in \mathbb{R}^{\mathcal{I}}, \tag{2.11}$$

while the spectral problem (2.9) is discretised as

$$\mathcal{L}U \equiv (\mathcal{A}+\mathcal{V})U = \lambda \mathcal{M}U, \quad U \in \mathbb{R}^{\mathcal{I}}, \tag{2.12}$$

where U denotes the vector representation of $u \in \mathbb{V}_n$ in the basis set $\{\phi_{\mathbf{i}}\}$. This leads to the explicit definition of the stiffness/mass matrices,

$$\langle \mathcal{A}U, V\rangle := \langle A\nabla u, \nabla v\rangle_{(L^2(\Omega))^d}, \quad \langle \mathcal{V}U, V\rangle := \langle Vu, v\rangle_{L^2(\Omega)}, \quad \langle \mathcal{M}U, V\rangle := \langle u, v\rangle_{L^2(\Omega)},$$

and the vector in the right-hand side,

$$\langle F, V\rangle := \langle f, v\rangle_{L^2(\Omega)}, \quad \forall u, v \in \mathbb{V}_n.$$

We follow the concept of approximate (truncated) iterations based on usage of the rank structured formats to represent matrix-vector operations in the framework of *preconditioned iterative solvers* (cf. [16, 14]).

For the linear system (2.11) the truncated preconditioned iteration takes the form

$$\widetilde{U}_{m+1} = U_m - \mathcal{B}^{-1}(\mathcal{A}U_m - F), \quad U^{(m+1)} := T_{\mathcal{S}}(\widetilde{U}^{(m+1)}),$$

where the truncation operator $T_{\mathcal{S}}$ is defined by the nonlinear approximation procedure that "projects" the respective vectors onto some manifold $\mathcal{S}$ of rank structured tensors.

In turn, solving the spectral problem (2.12) in the rank structured formats can be realised via the truncated preconditioned inverse iteration as follows,

$$\widetilde{U}_{m+1} = U_m - \mathcal{B}^{-1}(\mathcal{A}U_m - \mu_m U_m), \quad U^{(m+1)} := T_{\mathcal{S}}(\widetilde{U}^{(m+1)}),$$
$$U^{(m+1)} : U^{(m+1)}/\|U^{(m+1)}\|, \quad \mu_{m+1} = (\mathcal{A}U_{m+1}, U_{m+1}).$$

In both cases, the preconditioner $\mathcal{B}^{-1}$ can be chosen as inverse of the shifted Laplacian. In the following we present the more general construction of $\mathcal{B}$.

In the framework of FEM Galerkin equations (2.11) and (2.12) we introduce the class of elliptic operators which allow the low tensor rank approximate inverse. Let $\Sigma_0 : H_0^1(\Omega) \to H^{-1}(\Omega)$ be an elliptic operator given by the (positive) diagonal coefficients matrix $D = \mathrm{diag}\{D_1, ..., D_d\} \in C(\Omega; \mathbb{R}^{d\times d})$, and by the "univariate" potentials $V_\ell(x_\ell)$,

$$\Sigma_0 := -\sum_{\ell=1}^{d} \Sigma_\ell, \quad \text{with} \quad \Sigma_\ell = -\frac{d}{dx_\ell} D_\ell(x_\ell) \frac{d}{dx_\ell} + V_\ell(x_\ell), \quad \ell = 1, ..., d.$$

Suppose that the elliptic operator Σ_ℓ ($\ell = 1, ..., d$) is positive definite and let $\mathcal{A}_\ell \in \mathbb{R}^{n\times n}$ be the Galerkin discretisation of Σ_ℓ. Introduce the class of rank-R Kronecker product preconditioners defined by approximate inverse

$$\mathcal{B}_R \approx \mathcal{L}_0^{-1} \quad \text{with} \quad \mathcal{L}_0 := \mathcal{A}_1 \otimes ... \otimes I + ... + I \otimes ... \otimes \mathcal{A}_d.$$

Here the coefficients D_ℓ, V_ℓ can be chosen from the optimisation of the condition number in

$$C_1 \langle \mathcal{L}U, U\rangle \le \langle \mathcal{L}_0 U, U\rangle \le C_2 \langle \mathcal{L}U, U\rangle \quad \forall U \in \mathbb{V}_n, \tag{2.13}$$

so that the matrix $\mathcal{L}_0$ is supposed to be spectrally close/equivalent to the initial stiffness matrix $\mathcal{A} + \mathcal{V}$.

The construction of approximate inverse in the form of rank-R Kronecker tensor product representation is based on the *sinc*-quadrature method (see Lemma 3.2 below). In §3.1 we prove the spectral equivalence estimates for the preconditioner $\mathcal{B}_R$ and show that the storage requirement for the respective representation (3.1) is linear in d, $\mathcal{O}(dRn^q)$, with $q = 1, 2$ (compare with the linear complexity in the volume $N = n^d$).

Remark 2.2 *We notice that the potential function $V(x), x \in \mathbb{R}^d$, might include non-separable (singular) terms like $\sum_m 1/\|x - x_m\|$. The low tensor-rank approximation of a class of Green's kernels will be addressed in Section 2.4. Moreover, the tensor representation of the Schrödinger type operators was discussed in [3].*

2.4 Equations in unbounded domain and BEM applications

2.4.1 General discussion

In the case $\Omega = \mathbb{R}^d$, we set $A = I \in C(\Omega; \mathbb{R}^{d\times d})$, and consider the corresponding boundary value problem (BVP) and eigen-value problem (EVP) in the form

$$-\Delta u + Vu = f, \quad \text{and} \quad -\Delta u + Vu = \lambda u, \tag{2.14}$$

subject to the corresponding "radiation condition" as $\|x\| \to \infty$. There are several commonly used numerical methods for solving (2.14) based on the application of the fundamental solutions of related elliptic operators with constant coefficients:

1. Computation of particular solution (potential) by the convolution of the given right-hand side (density) with the related fundamental solution.
2. Boundary element methods (BEM) in bounded/unbounded domains.
3. Green function (fixed point) formulation of equations (2.14).

The reference elliptic operator with constant coefficients will be chosen as the shifted Laplacian,

$$-\Delta \pm z^2 I, \quad z \in [0, \infty).$$

Hence, in general, we are interested in the tensor-structured approximation of the respective elliptic resolvent (Green's function operator)

$$R_z := (-\Delta \pm z^2 I)^{-1}, \quad z \in [0, \infty)$$

with the kernel function defined by spherically symmetric fundamental solution (Green function) $G_z(x), x \in \mathbb{R}^d$. The fundamental solution of the operators $-\Delta$, and $-\Delta + z^2$, $Re\, z^2 > 0$, in $\mathbb{R}^d$ is given by

$$G_0(x) = \frac{\Gamma(\frac{d}{2} - 1)}{4\pi^{n/2}\|x\|^{n-2}}, \quad \text{and} \quad G_z(x) = \frac{1}{2\pi^{n/2}} \left(\frac{z}{\|x\|^{n-2}}\right)^{n/2-1} K_{n/2-1}(z\|x\|), \tag{2.15}$$

respectively, where K_ν is the modified Bessel function of the second kind [1, §9.6]. In turn, the fundamental solution of the Helmholtz type operator $\Delta + \kappa^2$, $\kappa^2 > 0$ takes the form

$$G_\kappa(x) = \frac{i}{4}\left(\frac{\kappa}{2\pi\|x\|}\right)^{n/2-1}, \quad x \in \mathbb{R}^d, H^{(1)}_{n/2-1}(\kappa\|x\|), \tag{2.16}$$

where $H^{(1)}_{n/2-1}$ is the Hankel function of the first kind [1]. In particular, in the case $d = 3$, the corresponding fundamental solution is given by the classical Newton ($z = 0$), Yukawa ($-\Delta + z^2, z > 0$) or Helmholtz ($\Delta + \kappa^2, \kappa > 0$) kernels,

$$G_0(x) := \frac{1}{4\pi}\frac{1}{\|x\|}, \quad G_z(x) := \frac{1}{4\pi}\frac{e^{-z\|x\|}}{\|x\|}, \quad G_\kappa(x) := \frac{1}{4\pi}\frac{e^{i\kappa\|x\|}}{\|x\|}, \quad x \in \mathbb{R}^3,$$

respectively.

The common feature of the family $G_z(\|x\|)$ is the analyticity in variable $\rho = \|x\|^2$, except the singularity point $\rho = 0$. This property together with spherical symmetry allows efficient separation of variables $x_1, ..., x_d$, in $\mathbb{R}^d$. In the case of non-oscillating kernels as in (2.15) the separable representation can be constructed by using the quadrature approximation of the Laplace transform,

$$G_z(\|x\|) = \int_{\mathbb{R}_+} \widehat{G}_z(t) e^{-t\|x\|^2} dt, \quad x \in \mathbb{R}^d.$$

For $d = 3$, the quadrature approximation of the Newton/Yukawa potentials $\frac{e^{-\kappa\sqrt{\rho}}}{\sqrt{\rho}}$ for $\kappa \in [0, \infty)$, is based on application of the *sinc*-quadratures to the Gauss transform

$$G(\rho) = \frac{e^{-\kappa\sqrt{\rho}}}{\sqrt{\rho}} = \frac{2}{\sqrt{\pi}} \int_{\mathbb{R}_+} exp(-\rho\tau^2 - \kappa^2/4\tau^2) d\tau, \quad \rho = \|x\|^2. \tag{2.17}$$

We are interested in the L^2-projection onto the set of tensor-product basis functions $\{\phi_{\mathbf{i}}\}$ introduced above (say, piecewise constant basis functions). The low tensor rank approximations for the arising d-th order coefficients tensor

$$\mathcal{G} = [G_{\mathbf{i}}]_{\mathbf{i}\in\mathcal{I}} \quad \text{with} \quad G_{\mathbf{i}} = \int G(\rho(x))\phi_{\mathbf{i}}(x) dx$$

is proven in [13, Lemma 4.3], [20, Theorem 3]:

Proposition 2.3 *The tensor $\mathcal{G} \in \mathbb{R}^{\mathcal{I}}$ allows the rank-R sinc-quadrature based approximation $\mathcal{G}_R \in \boldsymbol{\mathcal{C}}_{R,\mathbf{n}}$, such that*

$$\|\mathcal{G} - \mathcal{G}_R\| \le Ce^{-\beta R/\log R},$$

where constants C, β do not depend on R. The approximation error $\varepsilon > 0$ is achieved by the Tucker/canonical approximation with the rank estimate $r \le R \le O(|\log\varepsilon|)$ up to low order terms.

The numerical illustrations for $G_z(x)$ with $d = 3$ can be found in §3.4 (see also [2, 20]). Low rank representation of $G_z(x)$ can be utilised in fast tensor convolution transform [21, 22, 24]. Construction of separable approximation to non-oscillating fundamental solution G_z for $d > 3$ can be based on similar sinc-methods.

In the present paper, we focus on the important special case. Specifically, we consider separable approximation for the Helmholtz kernel $G_\kappa(x)$ for $d = 3$ and for its formal multidimensional counterpart given by the function $\frac{e^{i\kappa\|x\|}}{\|x\|}$, $\quad x \in \mathbb{R}^d$, $d > 3$ (though the latter does not represent the fundamental solution for the 3D Helmholtz operator in $\mathbb{R}^d$, our constructions can be useful for understanding the effects of higher dimensions). Our main result proves the rank-$O(\kappa)$ tensor approximation for the Helmholtz kernel that scales linearly in the frequency parameter κ (see Section 3.3). This result leads to sublinear cost $O(\kappa n \log n)$, regarded to $n \times n \times n$ spatial grids. Up to our best knowledge, low separation rank tensor approximation for oscillating kernels have not been yet addressed in the literature (cf. the asymptotically optimal methods in the volume size based on the fast multipole type representations [5, 6]).

In the next two subsections we discuss the particular numerical schemes for solving elliptic PDEs which can be gainfully improved by using tensor approximations to Green's functions.

2.4.2 Application in FEM-BEM coupling

Consider the FEM applications dealing with elliptic problems in unbounded domain. The initial BVP posed in $\Omega = \mathbb{R}^d$,

$$-\Delta u + Vu = f, \tag{2.18}$$

and subject to the corresponding radiation conditions as $\|x\| \to \infty$, can be reduced to the equation in the auxiliary bounded "tensor product" domain $\Omega_0 = [-a, a]^d$, $a > 0$, with the nonlocal boundary conditions posed on $\Gamma = \partial\Omega_0$. Specifically, assuming that $V(x) = const \geq 0$ and $f(x) = 0$, for $x \in \mathbb{R}^d \setminus \Omega_0$, and introducing the free-space Green's kernel $G(\|x-y\|)$ for the corresponding "external" elliptic operator with constant coefficients, the equation (2.18) can be rewritten in the form

$$-\Delta u + Vu = f \quad \text{in} \quad \Omega_0; \quad u - (I + \mathcal{K})^{-1}\mathcal{V}\partial_n u = 0 \quad \text{on} \quad \Gamma, \tag{2.19}$$

where the boundary Poincaré-Steklov (pseudo-differential) operator

$$\mathcal{S} = (I + \mathcal{K})^{-1}\mathcal{V} : H^{-1/2}(\Gamma) \to H^{1/2}(\Gamma),$$

is defined via the double layer and single layer integral operators $\mathcal{K}$ and $\mathcal{V}$ (see [25] for more details)

$$\mathcal{K}u = \int_\Gamma \partial_{n,y} G(\|x - y\|)u(y)dy, \quad \mathcal{V}u = \int_\Gamma G(\|x - y\|)u(y)dy, \tag{2.20}$$

with ∂_n beind the outward normal derivative on Γ. Hence, the tensor product representation of the integral operators $\mathcal{K}$ and $\mathcal{V}$ allows to implement the nonlocal boundary conditions (and the whole solution process) in the combined equation (2.19) using tensor product formats. In fact, if the the Green function $G(\|x\|)$ allows a tensor-structured representation on a tensor grid in $\mathbb{R}^d$, that geometrically fits the boundary Γ, then the action of the corresponding boundary integral operators in (2.20) can be implemented in tensor format as well, just by "tracing" the tensor product volume representation onto the piecewise tensor product boundary Γ. We will develop such tensor representations of the boundary (integral) operators elsewhere. In this way, the Poisson, Yukawa and Helmholtz type kernels in $\mathbb{R}^d$ can be adapted.

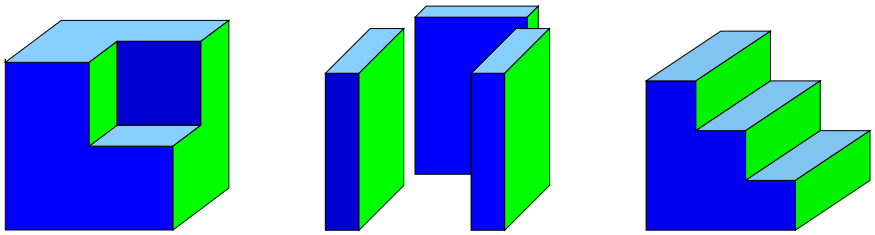

Figure 2.1: Examples of step-type 3D geometries.

The above strategy can be also extended to more complicated step-type geometries of Ω_0. Figure 2.1 represents examples of 3D piecewise tensor product geometries, which are well suited for tensor methods.

2.4.3 The Green function formulation

The Green function (fixed point) formulation applied to the spectral problems in quantum chemistry (the Lippmann-Schwinger equation) leads to the efficient numerical methods based on data-sparse representation of operators involved (see [17, 4] and references therein). This concept can be also applied as a preconditioning scheme for solving the elliptic boundary value problems.

The Green function formulations of the corresponding BVP and EVPs as in (2.14), can be derived by multiplication with the elliptic resolvent (Green's function operator) R_z. The corresponding integral (Green function) formulation of the elliptic BVP in the form $-\Delta u + Vu = f$, reads as

$$u = \mathcal{G}_z u + f \star G_z \tag{2.21}$$

with

$$\mathcal{G}_z u := [V_0 u] \star G_z \equiv R_z(V_0 u), \quad V_0 = z^2 - V, \quad R_z = (-\Delta + z^2)^{-1},$$

where $\star$ denotes the convolution product in $L^2(\mathbb{R}^d)$. Here the parameter $z^2 \geq 0$ can be specified via some optimisation criteria, however $z = 0$ will be the standard choice (convolution with the Poisson kernel).

Under certain assumptions, $\mathcal{G}_z$ can be proved to be the bounded operator in $L^2(\mathbb{R}^d)$ (see[4, 28]), that allows simple and robust iterative solution methods provided that the convolution transform can be computed in the efficient way (cf. [19]).

In the case of spectral problem with the negative target eigenvalue $\lambda < 0$, by setting $z = \sqrt{-\lambda}$, one obtains the integral formulation to the initial eigen-value problem

$$u = \mathcal{G}_z u \quad \text{with} \quad \mathcal{G}_z u = [V_0 u] * G_z. \tag{2.22}$$

The important feature of this formulation is that any eigenvalue-eigenfunction pair, (λ, u), (λ in the discrete spectrum), for the operator $-\Delta + V$ generates a fixed point solution of the problem (2.22) (cf. [17, 4, 20] for the case of Hartree-Fock, electronic Schrödinger and Kohn-Sham equations).

We point out that the integral representation $\mathcal{G}_z = (V_0 \cdot) \star G_z$ is computationally attractive due to the following gainful features (see [17, 28]):

- Simple collocation-type discretisation with discontinuous basis functions (L^2 setting).
- Existence of low-separation rank approximations to the operators V and G_z that allows fast tensor-product convolution transform.
- Robust and fast convergence of the nonlinear fixed point iterations to solve (2.21) and (2.22), which are well suited for the numerical multi-linear algebra via truncation to the prescribed tensor format.

For the rest of this section, we discuss in more detail the tensor approximation to the discrete convolution transform with the corresponding Green's kernels. Notice that the tensor-product multidimensional convolution for the class of translation invariant kernels was developed in [23, 21, 20]. In this way, we consider the collocation-type approximation of the operator $\mathcal{G}_z = (V_0\,\cdot)\star G_z$ with respect to the certain ansatz space $W = span\{\phi_{\mathbf{i}}\} \subset L^2(\mathbb{R}^d)$ of possibly discontinuous tensor-product basis functions as in (2.10). Letting

$$\psi = \sum_{\mathbf{i}\in\mathcal{I}} a_{\mathbf{i}}\phi_{\mathbf{i}}, \quad \mathbb{V}_0 = \{\langle V_0\phi_{\mathbf{i}}, \phi_{\mathbf{j}}\rangle\}_{\mathbf{i},\mathbf{j}\in\mathcal{I}} \in \mathbb{R}^{\mathcal{I}\times\mathcal{I}},$$

we calculate the L^2-projection $\mathcal{P}_W(V_0\psi)$ of $V_0\psi$ onto W,

$$\mathcal{P}_W(V_0\psi) = \sum_{\mathbf{j}\in\mathcal{I}}\sum_{\mathbf{i}\in\mathcal{I}} a_{\mathbf{i}}\langle V_0\phi_{\mathbf{i}}, \phi_{\mathbf{j}}\rangle\phi_{\mathbf{j}} = \sum_{\mathbf{j}\in\mathcal{I}} b_{\mathbf{j}}\phi_{\mathbf{j}}$$

with $b_{\mathbf{j}} = (\mathbb{V}_0\mathcal{A})_{\mathbf{j}}$, $\mathcal{A} = [a_{\mathbf{i}}]$. Introducing the coefficients tensor

$$\mathcal{B} = [b_{\mathbf{j}}]_{\mathbf{j}\in\mathcal{I}} \in \mathbb{R}^{\mathcal{I}}, \quad \text{i.e., } \mathcal{B} = \mathbb{V}_0\mathcal{A},$$

the discretisation of $\mathcal{G}_z\psi$ can be then defined by multidimensional convolution,

$$\mathcal{G}_z\psi \approx \mathcal{G}\star\mathcal{B},$$

where tensor $\mathcal{G}$ is obtained by the projection of the convolving kernel $G_z(x) = e^{-z\|x\|}/\|x\|$ onto the space W (see Proposition 2.3),

$$\mathcal{G} = [G_{\mathbf{i}}]_{\mathbf{i}\in\mathcal{I}} \quad \text{with} \quad G_{\mathbf{i}} = \int G_z(x)\phi_{\mathbf{i}}(x)dx.$$

In the case of piecewise constant basis functions in (2.10) the stiffness matrix $\mathbb{V}_0$ becomes diagonal, $\mathbb{V}_0 = diag\{\langle V_0\phi_{\mathbf{i}}, \phi_{\mathbf{i}}\rangle\}_{\mathbf{i}\in\mathcal{I}}$ (local operator of multiplication with $V_0(x)$). Here we presuppose the existence of low Kronecker rank representation for the matrix $\mathbb{V}_0$ as in (2.6). For example, this is the case if $V_0(x)$ is given by $\sum_\nu \frac{Z_\nu}{\|x-x_\nu\|} + g(x)$, with a smooth function g.

In some physical models solution (2.14) exhibits exponential decay as $\|x\| \to \infty$. In this case, the computational domain can be restricted to the fixed-size hypercube in $\mathbb{R}^d$. The similar situation arises in the traditional 3D BEM applications (see §2.4.2 above).

3 Low tensor rank preconditioners

3.1 Analysis of the preconditioner $\mathcal{B}_R$

We utilise the rank-R preconditioner $\mathcal{B}_R$ based on the sinc-quadrature approximation as follows,

$$\mathcal{B}_R := \sum_{k=-M}^{M} c_k \bigotimes_{\ell=1}^{d} \exp(-t_k \mathcal{A}_\ell) \approx \mathcal{L}_0^{-1}, \quad (t_k, c_k \in \mathbb{R}_+, \quad \mathcal{A}_\ell \in \mathbb{R}^{n\times n}). \tag{3.1}$$

It can be proven to provide exponential convergence in $R = 2M+1$ (see Lemma 3.2 below). Next simple lemma proves the linear scaling of the preconditioner $\mathcal{B}_R$ in d.

Lemma 3.1 *(Linear scaling). Preconditioner $\mathcal{B}_R$ in (3.1) has the Kronecker rank $R = 2M+1$, i.e. we have*

$$\mathcal{B}_R \in \boldsymbol{\mathcal{M}}_{R,\mathbf{n}}.$$

Let the operator coefficients D_ℓ, V_ℓ ($\ell = 1, ..., d$) be constant. Then the required storage and respective cost of the matrix-vector multiplication with rank-1 tensor can be estimated by

$$\mathcal{O}(dRn), \quad \textit{and} \quad \mathcal{O}(dRn\log n).$$

In the case of variable coefficients the related cost is bounded, respectively, by

$$\mathcal{O}(dRn^2), \quad \textit{and} \quad \mathcal{O}(dRn^2).$$

Proof. The Kronecker rank estimate is due to representation (3.1). Taking into account that in the case of constant coefficients the Galerkin matrix $\mathcal{A}_\ell$ ($\ell = 1, ..., d$) can be diagonalised at the cost $\mathcal{O}(n\log n)$ by using FFT matrices, we arrive at the linear-logarithmic scaling in n for the related matrix operations. The last assertion is due to the full format representation of the matrix exponential $exp(-t_k\mathcal{A}_\ell) \in \mathbb{R}^{n\times n}$ in the general case. ∎

To control the quality of preconditioning, we make use of the known error bound for the *sinc*-quadrature (3.1) applied to the Laplace transform of the matrix-valued function,

$$\mathcal{L}_0^{-1} = \int_0^\infty e^{-t\mathcal{L}_0} dt \quad \text{with} \quad cond(\mathcal{L}_0) = O(n^2).$$

The appropriate choice of quadrature parameters t_k, c_k (see (3.3)) leads to the exponential convergence rate (cf. [13, Lemma 4.3]),

$$\left\|\mathcal{L}_0^{-1} - \mathcal{B}_R\right\| \le C_0 e^{-\pi\sqrt{M}}, \tag{3.2}$$

where the constant $C_0 > 0$ does not depend on M and on n. Notice that the similar result was proven in [4, Theorem 22]. The following lemma proves the spectral equivalence estimates.

Lemma 3.2 *(Spectral equivalence). Let us set in (3.1)*

$$t_k = e^{k\mathfrak{h}}, \quad c_k = \mathfrak{h}t_k, \quad \mathfrak{h} = \pi/\sqrt{M}, \quad k = -M, ...M, \tag{3.3}$$

and suppose that the constants C_0, C_1, C_2 are determined by (3.2) and (2.13), respectively. Choose M such that the inequality $C_0\|\mathcal{L}_0\|\|\mathcal{B}_R^{-1}\|e^{-\pi\sqrt{M}} < q(M)C_1$ holds with $q < 1$, then we have

$$\widetilde{C}_1 \langle \mathcal{L}U, U\rangle \le \langle \mathcal{B}_R^{-1}U, U\rangle \le \widetilde{C}_2 \langle \mathcal{L}U, U\rangle \quad \forall U \in \mathbb{V}_n, \tag{3.4}$$

with spectral equivalence constants $\widetilde{C}_1, \widetilde{C}_2 > 0$ that allow the following bound on the condition number

$$\frac{\widetilde{C}_2}{\widetilde{C}_1} \le \frac{1}{1-q(M)}\frac{C_2}{C_1} + \frac{q(M)}{1-q(M)}.$$

Proof. The matrices $\mathcal{A}_\ell$, are symmetric and positive definite, hence, the Laplace transform and related exponential factors in (3.1) are correctly defined. Moreover, all terms in the sum $\mathcal{L}_0 = \mathcal{A}_1 \otimes ... \otimes I + ... + I \otimes ... \otimes \mathcal{A}_d$ mutually commute providing the corresponding factorisation of the matrix exponents $e^{-t_k\mathcal{L}_0} = \prod_{\ell=1}^{d} e^{-t_k I\otimes...\otimes\mathcal{A}_\ell\otimes...\otimes I}$ $(k = -M, ..., M)$. Then using the property of matrix exponential we obtain ,

$$\prod_{\ell=1}^{d} e^{-t_k I\otimes...\otimes\mathcal{A}_\ell\otimes...\otimes I} = \bigotimes_{\ell=1}^{d} e^{-t_k\mathcal{A}_\ell},$$

see [18, Theorem 5.3]. Moreover, we have

$$\left\|\mathcal{L}_0 - \mathcal{B}_R^{-1}\right\| = \left\|-\mathcal{L}_0(\mathcal{L}_0^{-1} - \mathcal{B}_R)\mathcal{B}_R^{-1}\right\| \le \|\mathcal{L}_0\| \left\|\mathcal{L}_0^{-1} - \mathcal{B}_R\right\| \left\|\mathcal{B}_R^{-1}\right\|.$$

Using (3.2) the constants $\widetilde{C}_1, \widetilde{C}_2 > 0$ can be estimated by

$$C_1 - C_0\|\mathcal{L}_0\|\|\mathcal{B}_R^{-1}\|e^{-\pi\sqrt{M}} \le \widetilde{C}_1, \quad \widetilde{C}_2 \le C_2 + C_0\|\mathcal{L}_0\|\|\mathcal{B}_R^{-1}\|e^{-\pi\sqrt{M}},$$

with $C_0 > 0$ defined in (3.2). Combining the above inequality with the error estimate (3.2) and with (2.13) leads to the desired bound. ∎

Remark 3.3 *Lemma 3.2 indicates that the Kronecker rank-R preconditioner $\mathcal{B}_R^{-1}$ has linear (or quadratic) scaling in the univariate problem size n, providing at the same time the condition number of order C_2/C_1 in (2.13), as soon as the estimate*

$$C_0\|\mathcal{L}_0\| \left\|\mathcal{B}_R^{-1}\right\| e^{-\pi\sqrt{M}} < C_1$$

holds. The latter is valid for $R = O(|\log(q(M)/C_1)|^2) = O((\log n)^2)$. Notice that the modified sinc-quadrature leads to the improved convergence rate in (3.2), $Ce^{-\alpha M/\log(M)}$ with $\alpha = \log(cond(\mathcal{L}_0))$ (cf. [18, Lemma 9.3], [13, Lemma 4.3]) again providing the rank estimate $R = O(\log(|\log(q(M))|/C_1)) = O((\log h)^2)$.

3.2 Canonical approximation of the oscillating Helmholtz kernels

We propose the construction of exponentially convergent tensor decompositions of the weakly singular oscillating kernels $\frac{e^{i\kappa\|x-y\|}}{\|x-y\|}$, $\kappa \in \mathbb{R}$, such that its real and imaginary parts

$$\frac{\cos(\kappa\|x-y\|)}{\|x-y\|} \quad \text{and} \quad \frac{\sin(\kappa\|x-y\|)}{\|x-y\|}, \quad x, y \in \mathbb{R}^d$$

will be treated separately. In the case $d = 3$, we obtain the rank-$O(\kappa)$ separable approximation for the oscillating Helmholtz kernel. At the end of Section 3 we provide numerical illustrations for $d = 3$, and for moderate $\kappa \leq 15$ which may substantiate the generic constants in the theoretical rank estimates.

On the first step, we transform the singular cos-kernel to the "more regular" kernel by subtraction of the principal singularity $\frac{1}{\|x\|}$. Then we construct separable approximations of the "regular" Helmholtz potentials

$$f_{1,\kappa}(\|x\|) := \frac{sin(\kappa\|x\|)}{\|x\|}; \quad f_{2,\kappa}(\|x\|) := \frac{1}{\|x\|} - \frac{cos(\kappa\|x\|)}{\|x\|} = \frac{2sin^2(\frac{\kappa}{2}\|x\|)}{\|x\|},$$

which leads to the respective approximations of the related kernel functions

$$f_{1,\kappa}(\|x-y\|), \quad f_{2,\kappa}(\|x-y\|), \quad x, y \in \mathbb{R}^d.$$

Figure 3.1 shows the complicated shape of the target functions $f_{1,\kappa}$ and $f_{2,\kappa}$ (2D slices of the potential in $d = 3$).

In the next statements we prove the rank estimates for the tensor approximations of both $f_{1,\kappa}$ and $f_{2,\kappa}$.

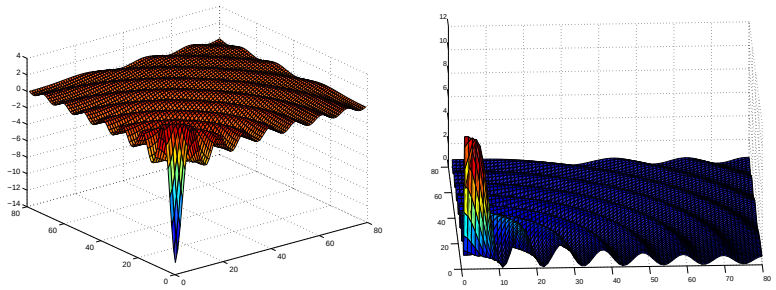

Figure 3.1: Visualisation of $f_{1,\kappa}$, $f_{2,\kappa}$ for $\kappa = 15$, $d = 3$.

Theorem 3.4 *For given tolerance $\varepsilon > 0$, the function $f_{1,\kappa} : [0, \frac{2\pi}{\sqrt{d}}]^d \to \mathbb{R}$ allows the Tucker/canonical approximations, such that*

$$\sigma(f_{1,\kappa}, \mathcal{S}) \leq C\varepsilon \quad with \quad \mathcal{S} = \{\boldsymbol{\mathcal{T}}_{\mathbf{r}}, \boldsymbol{\mathcal{C}}_R\},$$

and with the rank estimates ($\mathbf{r} = (r, ..., r)$),

$$r \leq R \leq Cd(|\log\varepsilon| + \kappa).$$

Proof. We set $t = \|x\|^2$ and then approximate the entire function $g(t) = \frac{sin(\kappa\sqrt{t})}{\sqrt{t}}$, $t \in [0, 2\pi]$ by trigonometric polynomials in t up to the accuracy ε in the max-norm. To that end we make use of the change of variables $z = \cos(t)$, $z \in [-1, 1]$, and consider the entire function $f(z) = g(arccos(z))$ that has the maximum value $O(e^\kappa)$ on the respective Bernstein's regularity ellipse of size $O(1)$. Applying the Chebyshev series to the function $f(z)$,

$$f(z) \approx C_0 + \sum_{m=1}^{M} C_m T_m(z), \quad z \in [-1, 1],$$

and taking into account that the Chebyshev polynomials satisfy $T_m(z) = cos(m\ arrcos\, z)$, $z \in [-1, 1]$, we are led to approximation by trigonometric polynomials (up to tolerance $\varepsilon > 0$) with $M = O(|\log \varepsilon| + \kappa)$ terms, where each trigonometric term has the form $\cos(mt) = \cos(m\|x\|^2)$.

Notice that the multivariate function $h(x) := \cos(x_1^2 + ... + x_d^2)$ has a separation rank $R \le d$, i.e. $h \in \mathcal{C}_R$, that is the consequence of the "magic" rank-d representation (cf. [3])

$$\sin(\sum_{i=1}^{d} x_j) = \sum_{i=1}^{d} \sin x_j \prod_{k \in \{1,...,d\} \setminus \{j\}} \frac{\sin(x_k + \alpha_k - \alpha_j)}{\sin(\alpha_k - \alpha_j)},$$

which is valid for all $\alpha_k \in \mathbb{R}$, such that $\sin(\alpha_k - \alpha_j) \neq 0$ for all $j \neq k$.

Now, the result follows by combination of the rank estimate for Chebyshev trigonometric approximation with the inclusion $h \in \mathcal{C}_R$. ■

Theorem 3.4 gives the constructive proof of the existence of low tensor rank approximation for the continuous function $f_{1,\kappa}$. Next statement applies to the d-th order tensor representing the projected kernel $f_{2,\kappa}$ onto the piecewise constant basis functions. Extension to the case of higher order tensor-product polynomials is straightforward. For further constructions, we introduce the function

$$f_1(t) := \frac{sin^2(\kappa/2\sqrt{t})}{t} \equiv \left(f_{1,\kappa/2}(t)\right)^2.$$

Theorem 3.5 *For given $\varepsilon > 0$, the coefficients tensor corresponding to $f_{2,\kappa} : [0, \frac{2\pi}{\sqrt{d}}]^d \to \mathbb{R}$,*

$$\mathcal{G} = [G_{\mathbf{i}}]_{\mathbf{i} \in \mathcal{I}} \quad with \quad G_{\mathbf{i}} = \|x_{\mathbf{i}}\| f_1(\|x_{\mathbf{i}}\|) \int_{\mathbb{R}^d} \frac{1}{\|x\|} \phi_{\mathbf{i}}(x) dx$$

allows the Tucker/canonical approximations, such that $\sigma(\mathcal{G}, \mathcal{S}) \le C\varepsilon \quad with \quad \mathcal{S} = \{\boldsymbol{\mathcal{T}}_{\mathbf{r}}, \boldsymbol{\mathcal{C}}_R\}$, and with the rank estimates,

$$r \le R \le Cd^2 |\log \varepsilon| \, (|\log \varepsilon| + \kappa) \quad (\mathbf{r} = (r, ..., r)).$$

The numerical complexity of the rank-R canonical approximation is bounded by

$$O(d^3 |\log \varepsilon| \, (|\log \varepsilon| + \kappa) n).$$

Proof. We factories the function $g(t) = \frac{sin^2(\kappa/2\sqrt{t})}{\sqrt{t}}$ (with $t = \|x\|^2 \in [0, 2\pi]$) as

$$g(t) = t \frac{1}{\sqrt{t}} f_1(t) \quad \text{with} \quad f_1(t) = \left(f_{1,\kappa/2}(t)\right)^2.$$

Now we apply the same argument as in Theorem 3.4 to the entire function $f_1 : [0, 2\pi] \to \mathbb{R}$ and obtain its separable approximation in classes $\boldsymbol{\mathcal{T}}_{\mathbf{r}}$ and $\boldsymbol{\mathcal{C}}_R$ (on the continuous level) that allows the κ-dependent rank estimate

$$r \le R \le Cd(|\log \varepsilon| + \kappa).$$

Since $f = t$ is the rank-d function of variables $(x_1, ..., x_d)$, we are left to the tensor approximation of the coefficients tensor for the Newton potential $1/\|x\|$ (see Proposition 2.3, [19,

Lemma 4.3] and [20, Theorem 3]). Using the rank-$|\log\varepsilon|$ approximation of the coefficients tensor for Newton potential, we arrive at the desired rank estimate for the resultant canonical tensor $[G_{\mathbf{i}}]_{\mathbf{i}\in\mathcal{I}}$ obtained as the Hadamard product of three canonical factors with respective rank parameters $d, |\log\varepsilon|$ and $d(|\log\varepsilon|+\kappa)$. ■

We comment that Theorems 3.4 and 3.5 indicate linear scaling of the tensor rank in the frequency parameter κ, which can lead to the remarkable reduction of the numerical cost in the case of moderate and high frequencies, $\kappa \le Cn$.

3.3 Complexity issues and numerics

Theorems 3.4 and 3.5 imply that the canonical tensor representation (up to tolerance $\varepsilon > 0$) of the descretized Helmholtz kernel on $n \times n \times n$ grid amounts to $O(|\log\varepsilon|(|\log\varepsilon|+\kappa)n)$ which allows the upper bound $O(|\log\varepsilon|n^2)$ for high frequency regime, $\kappa = Cn$.

Given the dimension parameter d and the univariate grid size n, we ask the question when the canonical format requires less storage than the orthogonal Tucker representation. The corresponding parameter relation is given by

$$dRn \le r^d + drn,$$

which leads to the condition that ensures the priority of the canonical representation,

$$d(\frac{R}{r} - 1)n \le r^{d-1}.$$

The latter will be always satisfied in higher dimensions.

In the case of traditional FEM/BEM applications, i.e., if $d = 3$, we set $\frac{R}{r} = 2$ (typical in our numerical practice), then we arrive at the priority relation for the canonical representation

$$\sqrt{3n} \le r,$$

which can be satisfied only on very coarse grids (recall that for non-oscillating kernels we have $r = O(\log n)$). However, for the case of oscillating kernels we may have $\kappa = Cn$, i.e., the canonical decomposition would be more preferable.

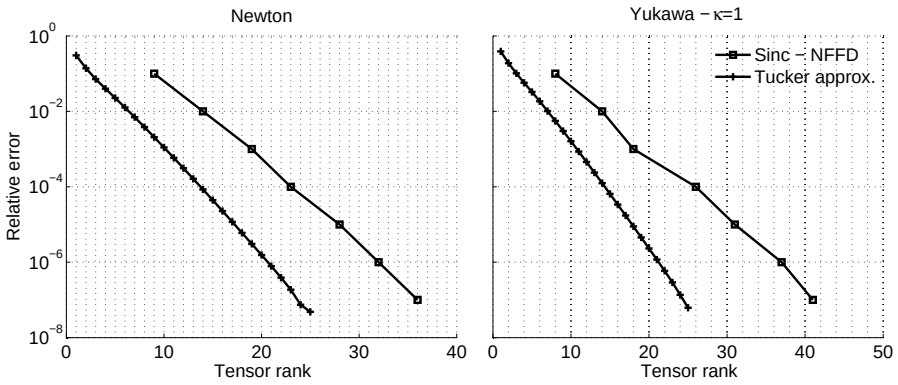

Figure 3.2: The Tucker vs. canonical approximation of the 3D Newton/Yukawa kernels.

Proceeding with the case of 3D Helmholtz kernel, we notice that $\kappa \leq Cn$ ensures that the Tucker model scales linear in $N_{vol} = n^3$. Furthermore, if $\kappa \leq Cn^{2/3}$ then the Tucker model scales sublinear in N_{vol} and linear in $N_{BEM} = n^2$. Recall that the approximation condition in the high-frequency domain is given by $\kappa \leq Cn$.

Below we present some numerical illustrations. The computations were performed in MATLAB 7.3.

Example 1. Figure 3.2 represents the convergence history for the best orthogonal Tucker [24] vs. canonical [2] approximations of the Newton/Yukawa potentials on $n \times n \times n$ grid for $n = 2048$.

Example 2. Figure 3.3 shows the convergence history for the Tucker model applied to $f_{1,\kappa}$, $f_{2,\kappa}$ depending on $\kappa \in [1, 15]$ and termination criterian with fixed values $\varepsilon_1 > 0$, and $\varepsilon_2 > 0$. It is clearly indicating the relation $r \sim C + \kappa$ for differen (fixed) values of $\varepsilon_1 = 10^{-3}$ and $\varepsilon_2 = 10^{-3}$.

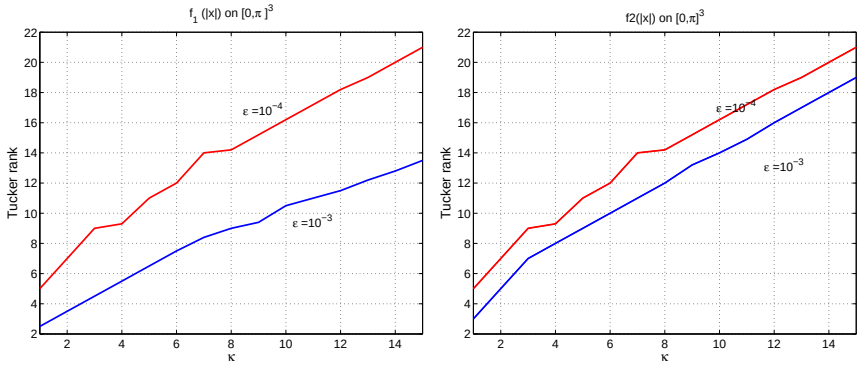

Figure 3.3: Convergence history for the Tucker model applied to $f_{1,\kappa}$, $f_{2,\kappa}$, $\kappa \in [1, 15]$.

Convergence for the Tucker and canonical models applied to $f_{2,\kappa}$, $\kappa \in [1, 15]$ is presented in Figures 3.4 and 3.5, respectively.

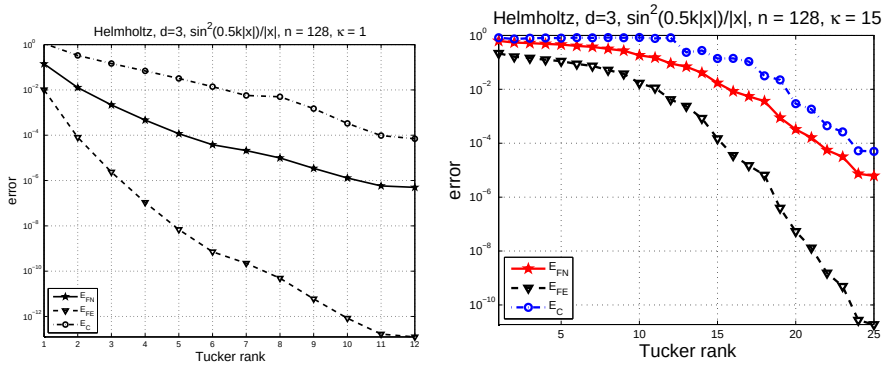

Figure 3.4: Convergence history for the Tucker model applied to $f_{2,\kappa}$, $\kappa \in [1, 15]$.

Figure 3.4,right clearly demonstrates exponential convergence in the Tucker rank r in the interval $r \geq r_0 = \kappa$ (supports the theory). We obtain the canonical approximation

(cf. Figure 3.5) by using the two-level format $\boldsymbol{\mathcal{T}}_{\mathcal{C}_{R,\mathbf{r}}}$, i.e., we compute the canonical rank-R decomposition by ALS-type iteration applied to the small-size $r \times r \times r$ Tucker core.

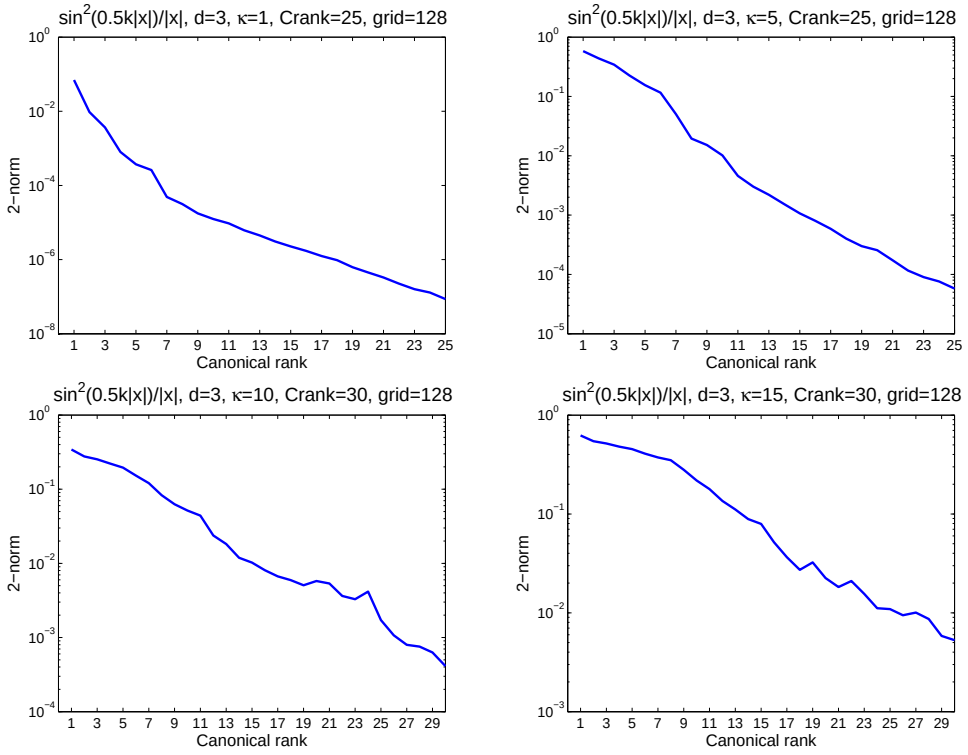

Figure 3.5: Convergence history for the canonical model applied to $f_{2,\kappa}$, $\kappa \in [1, 15]$.

Example 3. Results for canonical approximation of the Newton potential $1/\|x\|^{d-2}$, $x \in \mathbb{R}^d$, for $d = 3, 4, 5$, are depicted in Figure 3.6, while the respective convergence rate for weakly singular potential $1/\|x\|$, $d = 4, 5$ can be seen in Figure 3.7.

Example 4. Next Figure 3.8 indicates that the convergence of spectral (via trigonometric functions) approximations of the Helmholtz kernel deteriorates dramatically even for moderate frequences.

Example 5. Finally, we present the results on the iterative calculation of the minimal eigen-value for the d-dimensional finite difference Laplacian by power method with the rank truncation [14]. The rank-R tensor approximation is given by (3.1) with $\mathcal{A}_\ell = tridiag\{-1, 2, -1\} \in \mathbb{R}^{n\times n}$. Here, we discretise the problem on $(0, \pi)^d$ using n^d grid points and apply the *sinc*-quadrature with $M = 49$ to obtain the rank-$(2M + 1)$ appproximation of the Laplacian inverse for $d = 3, 10, 50$. The next table presents the computational time (sec.) per iteration, the relative H^1-error in the eigenfunction and the relative error in the eigen-value for $n = 2^9$. In all cases, the number of power iterations does not exceed 6.

This table clearly indicates the linear scaling in d of tensor-product approximation. More detailed numerical illustations on tensor-structured eigen-value solvers can be found in [14].

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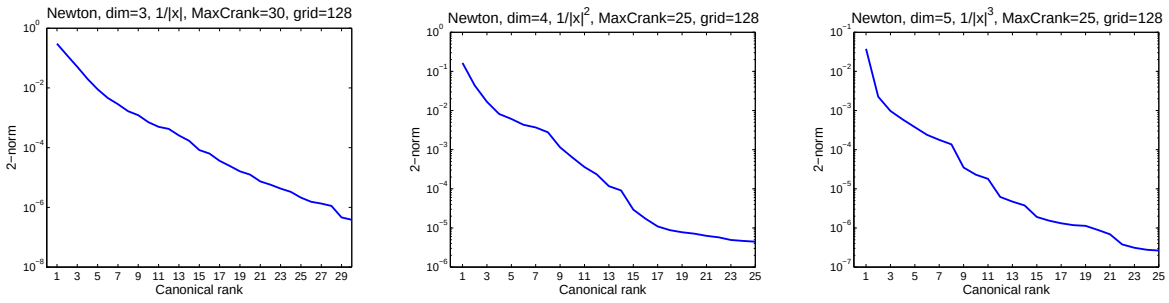

Figure 3.6: Canonical approximation applied to the Newton potential $1/\|x\|^{d-2}$ for $d = 3, 4, 5$.

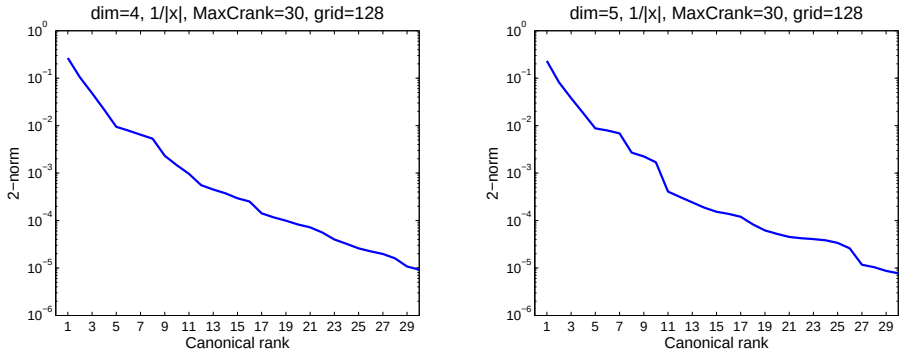

Figure 3.7: Canonical approximation applied to the weakly singular potential $1/\|x\|$ for $d = 4, 5$.

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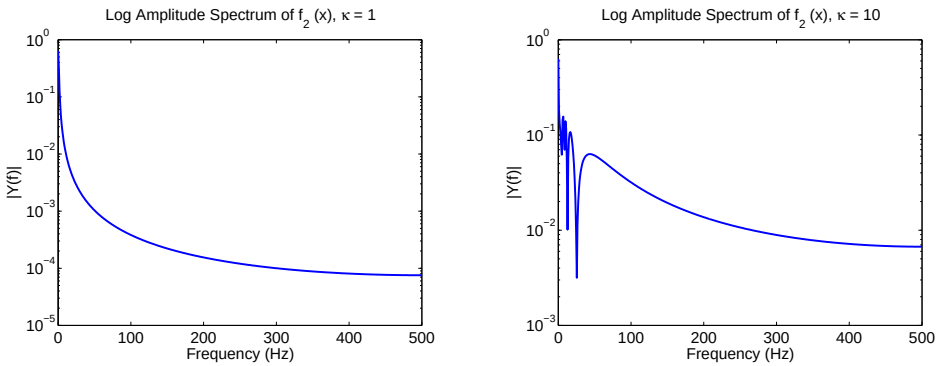

Figure 3.8: On spectral approximation of the Helmholtz kernel.

d	Time/it	δ_λ	δ_u
3	0.9	$3.1 \cdot 10^{-6}$	$4.5 \cdot 10^{-4}$
10	2.9	$3.1 \cdot 10^{-6}$	$3.8 \cdot 10^{-4}$
50	14.7	$3.1 \cdot 10^{-6}$	$3.1 \cdot 10^{-4}$

Table 3.1: Minimal eigen-value for the d-dimensional Laplacian ($d = 3, 10, 50$).

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