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**Low-Rank Kronecker-Product Approximation to
Multi-Dimensional Nonlocal Operators. Part I.
Separable Approximation of Multi-Variate
Functions**

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Low-Rank Kronecker-Product Approximation to Multi-Dimensional Nonlocal Operators. Part I. Separable Approximation of Multi-Variate Functions

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Abstract

The Kronecker tensor-product approximation combined with the \mathcal{H} -matrix techniques provides an efficient tool to represent integral operators as well as certain functions $F(A)$ of a discrete elliptic operator A in \mathbb{R}^d with a high spatial dimension d . In particular, we approximate the functions A^{-1} and $\text{sign}(A)$ of a finite difference discretisation $A \in \mathbb{R}^{N \times N}$ with a rather general location of the spectrum. The asymptotic complexity of our data-sparse representations can be estimated by $\mathcal{O}(n^p \log^q n)$, $p = 1, 2$, with q independent of d , where $n = N^{1/d}$ is the dimension of the discrete problem in *one* space direction. In this paper (Part I), we discuss several methods of a separable approximation of multi-variate functions. Such approximations provide the base for a tensor-product representation of operators. We discuss the asymptotically optimal *sinc* quadratures and *sinc* interpolation methods as well as the best approximations by exponential sums. These tools will be applied in Part II continuing this paper to the problems mentioned above.

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1 Introduction

In the wide range of applications the efficient numerical representation to certain multi-dimensional nonlocal operators posed in \mathbb{R}^d , $d \geq 2$, is needed. Examples of such nonlocal operators are multi-dimensional integral operators, solution operators of elliptic, parabolic and hyperbolic boundary value problems, Lyapunov and Riccati solution operators in control theory, spectral projection operators associated with the matrix *sign* function and the density matrix ansatz for solving the Schrödinger and Hartree-Fock equations, as well as collision integrals in the deterministic Boltzmann equation. As soon as computational issues are concerned, we are faced with the challenging problem of an accurate representation of large fully populated matrices or tensors (generally given only implicitly) in special data-sparse formats.

The class of *hierarchical* (\mathcal{H}) *matrices* allows an approximate matrix arithmetic with almost linear complexity [11]-[14], [9]. An \mathcal{H} -matrix approximation of the class of operator-valued functions of elliptic operators was developed in [4]-[6], [10]. For multi-dimensional problems, even approximations with linear complexity $\mathcal{O}(n^d)$ are not satisfactory due to the “curse of dimensionality”. To avoid an exponential scaling in d , one can try to represent the corresponding data (matrices and vectors) in a *tensor-product form* (cf. [1, 15, 19]) to reach the complexity $\mathcal{O}(dn^p \log^q n)$ ($p, q \geq 1$ independent of d). To decrease the exponent p , we use the hierarchical format for each factor, reducing the cost to $\mathcal{O}(dn \log^q n)$.

In [7], the \mathcal{H} -matrix techniques combined with the Kronecker tensor-product approximation (cf. [15, 19]) were applied to represent the inverse of a discrete elliptic operator in a hypercube $(0, 1)^d \in \mathbb{R}^d$. We recall that the *hierarchical Kronecker tensor-product* (HKT) approximation of a matrix is defined as follows. Given

a matrix $A \in \mathbb{C}^{N \times N}$ of dimension $N = n^d$, we approximate A by a matrix $A_{(r)}$ of the form

$$A_{(r)} = \sum_{k=1}^r V_k^1 \otimes \cdots \otimes V_k^d \approx A, \quad (1.1)$$

where the V_k^ℓ are $n \times n$ -matrices and \otimes denotes the Kronecker product operation. The crucial parameter is r , the number of products in (1.1), called the *Kronecker rank* (cf. [15]). Furthermore, each Kronecker factor V_k^ℓ is supposed to be represented in the \mathcal{H} -matrix form. The complexity of the HKT approximation can be estimated by $\mathcal{O}(dn \log^q n)$, where q is some fixed constant independent of d . Rank-one approximations of high-order tensors are, e.g., discussed in [23].

The HKT approximation of integral operators posed in \mathbb{R}^d is well understood, since it can be reduced to the separable approximation of the explicitly given kernel function together with an \mathcal{H} -matrix representation of the factors V_k^ℓ (cf. [15] related to the case $d = 2$). In Part II of this paper, we address this topic in the case of rather general shift-invariant kernel functions with $d \geq 2$.

A broad class of nonlocal operators in mathematical physics can be described by operator-valued functions of an elliptic operator. Concerning the elliptic operator \mathcal{A} given in the form

$$\mathcal{A} = - \sum_{j=1}^d \frac{\partial}{\partial x_j} a_j(x) \frac{\partial}{\partial x_j} + \sum_{j=1}^d b_j(x) \frac{\partial}{\partial x_j} + c(x), \quad x = (x_1, \dots, x_d) \in (0, 1)^d,$$

we further assume

$$a_j(x) = a_j(x_j), \quad b_j(x) = b_j(x_j) \quad \text{and} \quad c(x) = c_1(x_1) + \dots + c_d(x_d).$$

To derive the tensor-product representation, we employ a finite difference discretisation A of \mathcal{A} (e.g., a three-point stencil in each variable) using a uniform tensor-product grid in \mathbb{R}^d with n grid points in each spatial direction. We are considering a matrix-valued function $F(A)$ based on some integral representation. For instance, a negative fractional power of a positive definite matrix A can be represented by the integral

$$A^{-\sigma} = \frac{1}{\Gamma(\sigma)} \int_0^\infty t^{\sigma-1} e^{-tA} dt \quad (\sigma > 0) \quad (1.2)$$

(cf. [7]), provided that the integral exists. The discretisation matrix has the form $A = \sum_{j=1}^d A_j$ with $A, A_j \in \mathbb{R}^{N \times N}$, $N = n^d$, where the matrices A_j are mutually commutable.

We apply an exponentially convergent quadrature rule to represent the integral (1.2) by a sum involving only factorised expressions,

$$A^{-\sigma} \approx \sum_{k=-M}^M c_k t_k^{\sigma-1} \prod_{j=1}^d \exp(-t_k A_j), \quad (t_k, c_k \in \mathbb{R} \text{ quadrature points and weights}),$$

which leads to the desired HKT representation.

Remark 1.1 *Note that with the choice $\mathcal{A} = -\Delta$, the representation (1.1) is of particular interest in the cases $\sigma = 1/2$ (preconditioner of the Laplace-Beltrami operator $(-\Delta)^{1/2}$, and for hypersingular integral operators, e.g., in BEM applications), $\sigma = 1$ (inverse Laplacian), and $\sigma = 2$ (preconditioner for the biharmonic operator).*

There is a large class of matrix-valued functions $F(A)$ that can be approximated directly by exponential sums,

$$F_r(A) := \sum_{k=1}^r c_k \exp(t_k A) \approx F(A), \quad c_k \in \mathbb{R}, \quad (1.3)$$

such that r grows only logarithmically with respect to the desired accuracy. Then the separability property of exponentials can be easily adapted.

In some cases the approximation by exponential sums can be constructed by using some intermediate integral representations involving operator resolvents. The construction of an HKT approximation of the

inverse matrix and, in particular, of resolvents $(zI - A)^{-1}$, $z \in \mathbb{C}$, allows to approximate a rather general class of matrix-valued analytic functions, which can be represented by the Dunford-Cauchy integral, which, in turn, can be approximated by a quadrature formula

$$F(A) := \frac{1}{2\pi i} \int_{\Gamma} F(z)(zI - A)^{-1} dz \approx \sum_{k=-M}^M c_k F(z_k)(z_k I - A)^{-1}, \quad (1.4)$$

where Γ is a curve containing the spectrum of A .

For the particular matrix-valued function $F(A) = \text{sign}(A)$ (see Part II of this paper), a tensor-product representation can be based on an efficient quadrature for the integral

$$\text{sign}(A) = \frac{1}{c_F} \int_{\mathbb{R}_+} \frac{F(tA)}{t} dt \quad (1.5)$$

with certain functions F (say, with $F(t) = t \exp(-t^2)$ or with $F(t) = \frac{\sin(t) - t \cos(t)}{t^2}$).

Keeping in mind the above arguments, in this paper we focus on the construction of efficient quadratures for a class of (improper) integrals as well as on the approximation of analytic functions by exponential sums.

2 Sinc Interpolation and Quadrature

2.1 Separation by Integration

If a function of ρ can be written as the integral

$$\varphi(\rho) = \int_{\Omega} e^{\rho F(t)} G(t) dt$$

over some $\Omega \subset \mathbb{R}$ and if quadrature can be applied, one obtains $\varphi(\rho) \approx \sum_{\nu} \omega_{\nu} e^{\rho F(x_{\nu})} G(x_{\nu})$. Setting $\rho = \sum_{i=1}^d x_i$, we get the separable approximation

$$\varphi(x_1 + \dots + x_d) \approx \sum_{\nu} c_{\nu} \prod_{i=1}^d e^{x_i F(x_{\nu})}, \quad c_{\nu} = \omega_{\nu} G(x_{\nu}).$$

The above argument applies as well for the matrix-valued function $\varphi(A)$ with $A = \sum_{i=1}^d A_i$ and pairwise commutable matrices A_i . In §2.2 we discuss the Sinc quadrature in the case of $\Omega = \mathbb{R}$ and study the quadrature error. If the integration domain Ω is different from \mathbb{R} , one has first to apply a suitable substitution.

On the other hand, the best approximation of $\varphi(\rho)$ by exponential sums,

$$\varphi(\rho) \approx \sum_{\nu} c_{\nu} e^{-\omega_{\nu} \rho} \quad (2.1)$$

(e.g., with respect to the maximum norm), leads to an approximation whose separation rank is expected to be close to optimal.

2.2 Definitions

In this section, we present Sinc quadrature rules for computing the integral

$$I(f) = \int_{\Omega} f(\xi) d\xi \quad (\Omega = \mathbb{R} \text{ or } \Omega = \mathbb{R}_+). \quad (2.2)$$

In the case of $\Omega = \mathbb{R}$, following [5], $H^1(D_{\delta})$ is the set of all complex-valued functions f , which are analytic in the strip $D_{\delta} := \{z \in \mathbb{C} : |\Im z| \leq \delta\}$ with some $\delta < \frac{\pi}{2}$, such that

$$N(f, D_{\delta}) := \int_{\partial D_{\delta}} |f(z)| |dz| = \int_{\mathbb{R}} (|f(x + i\delta)| + |f(x - i\delta)|) dx < \infty.$$

Let

$$S(k, \mathfrak{h})(x) = \frac{\sin[\pi(x - k\mathfrak{h})/\mathfrak{h}]}{\pi(x - k\mathfrak{h})/\mathfrak{h}} \quad (k \in \mathbb{Z}, \mathfrak{h} > 0, x \in \mathbb{R}) \quad (2.3)$$

be the k -th Sinc function with step size \mathfrak{h} , evaluated at x . Given $f \in H^1(D_\delta)$, $\mathfrak{h} > 0$, and $M \in \mathbb{N}_0$, the corresponding Sinc interpolant (cardinal series representation) reads as

$$C(f, \mathfrak{h}) = \sum_{\nu=-\infty}^{\infty} S(\nu, \mathfrak{h})f(\nu\mathfrak{h}).$$

We use the conventional notations

$$\begin{aligned} C_M(f, \mathfrak{h}) &= \sum_{\nu=-M}^M S(\nu, \mathfrak{h})f(\nu\mathfrak{h}), & E_M(f, \mathfrak{h}) &= f - C_M(f, \mathfrak{h}), \\ T(f, \mathfrak{h}) &= \mathfrak{h} \sum_{k=-\infty}^{\infty} f(k\mathfrak{h}), & T_M(f, \mathfrak{h}) &= \mathfrak{h} \sum_{k=-M}^M f(k\mathfrak{h}), \\ \eta(f, \mathfrak{h}) &= I(f) - T(f, \mathfrak{h}), & \eta_M(f, \mathfrak{h}) &= I(f) - T_M(f, \mathfrak{h}). \end{aligned} \quad (2.4)$$

Here $\eta(f, \mathfrak{h})$ represents the quadrature error via the Sinc interpolant $C(f, \mathfrak{h})$,

$$\int_{\mathbb{R}} f(\xi)d\xi \approx \int_{\mathbb{R}} \sum_{\nu=-\infty}^{\infty} S(\nu, \mathfrak{h})f(\nu\mathfrak{h})d\xi = T(f, \mathfrak{h}),$$

and $\eta_M(f, \mathfrak{h})$ includes in addition the corresponding truncation error $T(f, \mathfrak{h}) - T_M(f, \mathfrak{h})$, while $E_M(f, \mathfrak{h})$ describes the interpolation error by the truncated Sinc interpolant.

2.3 Standard Error Estimates

If $f \in H^1(D_\delta)$ and

$$|f(\xi)| \leq C \exp(-b|\xi|) \quad \text{for all } \xi \in \mathbb{R} \text{ with } b, C > 0, \quad (2.5)$$

then the quadrature error η_M from (2.4) satisfies

$$|\eta_M(f, \mathfrak{h})| \leq C \left[\frac{e^{-2\pi\delta/\mathfrak{h}}}{1 - e^{-2\pi\delta/\mathfrak{h}}} N(f, D_\delta) + \frac{1}{b} \exp(-b\mathfrak{h}M) \right] \quad (2.6)$$

(cf. [18]). Furthermore, under the same assumptions on $f \in H^1(D_\delta)$, the interpolation error is bounded by

$$\|E_M(f, \mathfrak{h})\|_\infty \leq C \left[\frac{e^{-\pi\delta/\mathfrak{h}}}{2\pi\delta} N(f, D_\delta) + \frac{1}{b\mathfrak{h}} \exp(-b\mathfrak{h}M) \right]. \quad (2.7)$$

Equalising both terms in (2.6) or (2.7) leads us to the following result. In the case of (2.6), the choice $\mathfrak{h} = \sqrt{2\pi\delta/bM}$ yields the exponential convergence rate

$$|\eta_M(f, \mathfrak{h})| \leq Ce^{-\sqrt{2\pi\delta bM}} \quad (2.8)$$

with a positive constant C independent of M , depending only on f, δ, b (cf. [18, 5, 6]). Note that $2M + 1$ is the number of quadrature points. If f is an even function, the number of quadrature points reduces to $M + 1$.

In the case of (2.7), the choice $\mathfrak{h} = \sqrt{\pi\delta/bM}$ implies

$$\|E_M(f, \mathfrak{h})\|_\infty \leq CM^{1/2}e^{-\sqrt{\pi\delta bM}} \quad (2.9)$$

with a positive constant C depending only on f, δ, b (cf. [18]).

In the case $\Omega = \mathbb{R}_+$ one has to substitute the integral (2.2) by $\xi = \varphi(\zeta)$ such that $\varphi : \mathbb{R} \rightarrow \mathbb{R}_+$ is a bijection. This changes the integrand f into $f_1 := \varphi' \cdot (f \circ \varphi)$. Assuming $f_1 \in H^1(D_\delta)$, $I(f_1)$ is now defined for $\Omega = \mathbb{R}$ and one can apply (2.5)-(2.8) to the transformed function.

2.4 Improved Quadrature Error Estimates

The error estimate in (2.8) has an exponent involving \sqrt{M} . Under stronger assumptions it is possible to improve \sqrt{M} to $M/\log M$ as we show next (see [6] for a proof).

Proposition 2.1 *Let $f \in H^1(D_\delta)$ with some $\delta < \frac{\pi}{2}$. If f satisfies the stronger condition*

$$|f(\xi)| \leq C \exp(-be^{a|\xi|}) \quad \text{for all } \xi \in \mathbb{R} \quad \text{with } a, b, C > 0 \quad (2.10)$$

instead of (2.5), then the error η_M of $T_M(f, \mathfrak{h})$ satisfies

$$|\eta_M(f, \mathfrak{h})| \leq C \left[\frac{e^{-2\pi\delta/\mathfrak{h}}}{1 - e^{-2\pi\delta/\mathfrak{h}}} N(f, D_\delta) + \frac{e^{-a\mathfrak{h}M}}{ab} \exp(-be^{a\mathfrak{h}M}) \right].$$

The choice $\mathfrak{h} = \log(\frac{2\pi aM}{b}) / (aM)$ leads to

$$|\eta_M(f, \mathfrak{h})| \leq C N(f, D_\delta) e^{-2\pi\delta aM / \log(2\pi aM/b)}. \quad (2.11)$$

Remark 2.2 *Let $f \in H^1(D_\delta)$. Note that the quadratures from §2.3 and §2.4 apply also to matrix-valued functions $f(\xi) = F(\xi; A)$, in particular, to functions leading to A^{-1} , e.g., (1.2), (1.5) (see numerics in Section 5). In the case of diagonalisable matrices, the error analysis for the corresponding quadratures applied to $F(\xi; A)$ is similar to the analysis of parameter dependent scalar functions $f(\xi; \rho)$, where $\rho \in \sigma(A)$ (cf. [6, 7]). For the class of analytic functions of A , which can be represented by the Dunford-Cauchy integral (1.4), the analysis is analogous.*

In the following Sections 4-5, we take a closer look to two integrals of real functions, which are transformed in such a way that either (2.8) or (2.11) hold.

2.5 Improved Interpolation Error Estimates

Assuming the faster decay rate (2.10) of f , it is possible to improve the estimates (2.7) and (2.9).

Proposition 2.3 *Let $f \in H^1(D_\delta)$ with some $\delta < \frac{\pi}{2}$. If f satisfies (2.10), then the interpolation error E_M of $C_M(f, \mathfrak{h})$ satisfies*

$$\|E_M(f, \mathfrak{h})\|_\infty \leq C \left[\frac{e^{-\pi\delta/\mathfrak{h}}}{2\pi\delta} N(f, D_\delta) + \frac{e^{-a\mathfrak{h}M}}{ab\mathfrak{h}} \exp(-be^{a\mathfrak{h}M}) \right]. \quad (2.12)$$

The choice $\mathfrak{h} = \log(\frac{\pi aM}{b}) / (aM)$ leads to

$$\|E_M(f, \mathfrak{h})\|_\infty \leq C (1 + o(1)) \frac{N(f, D_\delta)}{2\pi\delta} e^{-\pi\delta aM / \log(\pi aM/b)}. \quad (2.13)$$

Proof. The error $E(f, \mathfrak{h}) := f - C(f, \mathfrak{h})$ allows the same estimate as in the standard case (see first term in the right-hand side of (2.7)),

$$\|E(f, \mathfrak{h})\|_\infty \leq C \frac{e^{-\pi\delta/\mathfrak{h}}}{2\pi\delta} N(f, D_\delta). \quad (2.14)$$

The truncation error bound hinges only upon the decay rate in (2.10),

$$\|C(f, \mathfrak{h}) - C_M(f, \mathfrak{h})\|_\infty \leq \sum_{|k| \geq M+1} |f(k\mathfrak{h})| \leq 2C \sum_{k=M+1}^{\infty} e^{-be^{ak\mathfrak{h}}} \leq \frac{2C}{ba\mathfrak{h}e^{a\mathfrak{h}M}} e^{-be^{a\mathfrak{h}M}}, \quad (2.15)$$

which proves the second term in the right-hand side of (2.12). For the chosen \mathfrak{h} , the first term in the right-hand side in (2.12) dominates, hence (2.13) follows. \blacksquare

For applications in finite element (FEM) and boundary element methods (BEM), we reformulate the previous result for parameter-dependent functions $g(x, y)$, $y \in Y \subset \mathbb{R}^m$, defined on the reference interval $x \in (0, 1]$. Following the approach in [16], we introduce the mapping

$$\zeta \in D_\delta \mapsto \phi(\zeta) = \frac{1}{\cosh(\sinh(\zeta))}, \quad \delta < \frac{\pi}{2}. \quad (2.16)$$

Clearly, $(0, 1] = \phi(\mathbb{R})$ and, moreover, $\phi(\zeta)$ decays twice exponentially,

$$|\phi(\zeta)| \leq 2 \exp\left(-\frac{\cos \delta}{2} e^{|\Re \zeta|}\right), \quad \zeta \in D_\delta.$$

In particular, we have $|\phi(\zeta)| \leq 2 \exp(-\frac{\cos \delta}{2} e^{|\zeta|})$ for $\zeta \in \mathbb{R}$. Let

$$D_\phi(\delta) := \{\phi(\zeta) : \zeta \in D_\delta\} \supset (0, 1] \quad (2.17)$$

be the image of D_δ . One checks easily that $D_\phi(\delta) \subset S_r(0) \setminus \{0\}$, where $S_r(0)$ is the disc around zero with a certain radius $r > 1$. Therefore, if a function g is holomorphic on $D_\phi(\delta)$, then

$$f(\zeta) := \phi^\alpha(\zeta)g(\phi(\zeta)) \quad \text{for any } \alpha > 0$$

is also holomorphic on D_δ .

Note that the finite Sinc interpolation $C_M(f(\cdot, y), \mathfrak{h}) = \sum_{k=-M}^M f(k\mathfrak{h}, y)S_{k,\mathfrak{h}}$ together with the back-transformation $\zeta = \phi^{-1}(x) = \operatorname{arsinh}(\operatorname{arcosh}(\frac{1}{x}))$ and multiplication by $x^{-\alpha}$ yields the separable approximation

$$g_M(x, y) := \sum_{k=-M}^M \phi(k\mathfrak{h})^\alpha g(\phi(k\mathfrak{h}), y) \cdot x^{-\alpha} S_{k,\mathfrak{h}}(\phi^{-1}(x)) \approx g(x, y) \quad (2.18)$$

of the function $g(x, y)$ for $x \in (0, 1] = \phi(\mathbb{R})$ and $y \in Y$. Since $\phi(\zeta)$ is an even function, the separation rank in (2.18) is reduced to $r = M + 1$. The error analysis is given by the following statement.

Corollary 2.4 *Let $Y \subset \mathbb{R}^m$ be any parameter set and assume that for all $y \in Y$ the functions $g(\cdot, y)$ together with their transformed counterparts $f(\zeta, y) := \phi^\alpha(\zeta)g(\phi(\zeta), y)$ satisfy the following conditions:*

- (a) $g(\cdot, y)$ is holomorphic on $D_\phi(\delta)$, and $\sup_{y \in Y} N(f(\cdot, y), D_\delta) < \infty$;
- (b) $f(\cdot, y)$ satisfies (2.10) with $a = 1$ and with certain C, b for all $y \in Y$.

Then, for all $y \in Y$, the optimal choice $\mathfrak{h} := \frac{\log M}{M}$ of the step size yields the pointwise error estimates

$$|E_M(f(\cdot, y), \mathfrak{h})| = |f(\zeta, y) - C_M(f(\cdot, y), \mathfrak{h})(\zeta)| \leq C \frac{N(f(\cdot, y), D_\delta)}{2\pi\delta} e^{-\pi\delta M / \log M}, \quad (2.19)$$

$$|g(x, y) - g_M(x, y)| \leq |x|^{-\alpha} |E_M(f(\cdot, y), \mathfrak{h})(\phi^{-1}(x))|. \quad (2.20)$$

Proof. Due to the properties of $\phi : D_\delta \rightarrow D_\phi(\delta)$, condition (a) implies $f \in H^1(D_\delta)$, hence, in view of (b), we can apply Proposition 2.3. Now $\frac{N(f, D_\delta)}{2\pi\delta} e^{-\pi\delta M / \log M}$ corresponds to (2.14), while the evaluation of (2.15) for the present \mathfrak{h} yields the bound $\frac{2C}{b \log M} e^{-bM}$, which is asymptotically faster decaying as $M \rightarrow \infty$.

The approximant (2.18) implies the bound (2.20) for $g - g_M(x, y)$. ■

The singularity at $x = 0$ is avoided by restricting x to $[h, 1]$ ($h > 0$). In applications with a discretisation step size h it suffices to apply this estimate for $|x| \geq \text{const} \cdot h$. Since usually $1/h = \mathcal{O}(n^\beta)$ for some β (and n the problem dimension), the factor $|x|^{-\alpha}$ is bounded by $\mathcal{O}(n^{\alpha\beta})$ and can be compensated by the exponential decay in (2.19) with respect to M . Note that Remark 2.2 remains valid here.

Corollary 2.4 and estimate (2.20) will be applied in Section 6.

2.6 Sinc Interpolation of Multi-Variate Functions

Given a multi-variate function $F : \mathbb{R}^d \rightarrow \mathbb{R}$ ($d \geq 1$), we are interested in its approximation by a separable expansion of the form

$$F_r(\zeta_1, \dots, \zeta_d) := \sum_{k=1}^r \Phi_k^1(\zeta_1) \cdots \Phi_k^d(\zeta_d) \approx F,$$

where the set of univariate functions $\{\Phi_k^\ell(\cdot) : 1 \leq \ell \leq d, 1 \leq k \leq r\}$ may be fixed or chosen adaptively (see the discussion in [1, 15, 19]). For numerical efficiency the so-called *separation rank* r should be reasonably small.

Next, we introduce the *tensor-product Sinc interpolation* \mathbf{C}_M with respect to the first $d - 1$ variables,

$$\mathbf{C}_M F := C_M^1 \dots C_M^{d-1} F,$$

where $C_M^\ell F = C_M^\ell(F, \mathfrak{h})$ denotes the univariate Sinc interpolation from (2.4) applied to the variable $\zeta_\ell \in I_\ell$. Here, $I_\ell = \mathbb{R}$ is the ℓ -th factor in $\mathbb{R}^d = I_1 \times \dots \times I_d$. For each fixed $\ell \in \{1, \dots, d - 1\}$, choose the variable ζ_ℓ and define the remaining parameter set by $Y_\ell := I_1 \times \dots \times I_{\ell-1} \times I_{\ell+1} \times \dots \times I_d \in \mathbb{R}^{d-1}$. This defines the univariate parameter-dependent function $F_\ell(\cdot, y) : I_\ell \rightarrow \mathbb{R}$, which is the restriction of F onto the interval I_ℓ with fixed parameter $y \in Y_\ell$. The estimation of the error $F - \mathbf{C}_M F$ requires the so-called Lebesgue constant $\Lambda_M \geq 1$ characterised by

$$\|C_M(f, \mathfrak{h})\|_\infty \leq \Lambda_M \|f\|_\infty \quad \text{for all } f \in C(\mathbb{R}). \quad (2.21)$$

Stenger [18, p. 142] proves the inequality

$$\Lambda_M = \max_{x \in \mathbb{R}} \sum_{k=-M}^M |S(k, \mathfrak{h})(x)| \leq \frac{2}{\pi} \left(\frac{3}{2} + \gamma + \log(M + 1) \right) \leq \frac{2}{\pi} (3 + \log(M)) \quad (2.22)$$

with Euler's constant $\gamma = 0.577\dots$. Note that we also have

$$\sum_{k=-\infty}^{\infty} |S(k, \mathfrak{h})(x)|^2 = 1 \quad (x \in \mathbb{R})$$

(cf. [18, p. 142]), which indicates $\Lambda_M = 1$ with respect to the L^2 -norm in (2.21) instead of the L^∞ -norm. Now we are able to prove the counterpart of Proposition 2.3 for the multi-variate interpolation error, which now is denoted by

$$\mathbf{E}_M(F, \mathfrak{h}) = F - \mathbf{C}_M(F, \mathfrak{h}).$$

Proposition 2.5 *For each $\ell = 1, \dots, d - 1$ we assume that for any $y_\ell \in Y_\ell$ the functions $F_\ell(\cdot, y_\ell)$ satisfy the following conditions:*

(a) $F_\ell(\cdot, y_\ell) \in H^1(D_\delta)$ with $N(F_\ell(\cdot, y_\ell), D_\delta) < \infty$ uniformly in $y_\ell \in Y_\ell$;

(b) $F_\ell(\cdot, y_\ell)$ satisfies (2.10) with $a = 1$ and with certain C, b for all $y_\ell \in Y_\ell$.

Then, for all $y_\ell \in Y_\ell$, the optimal choice $\mathfrak{h} := \frac{\log M}{M}$ of the step size yields the pointwise error estimate

$$|\mathbf{E}_M(F, \mathfrak{h})(\zeta)| = |F(\zeta) - \mathbf{C}_M(F, \mathfrak{h})(\zeta)| \leq \frac{C \Lambda_M^{d-1}}{2\pi\delta} \max_{\ell=1, \dots, d-1} N(F_\ell(\cdot, y_\ell), D_\delta) e^{\frac{-\pi\delta M}{\log M}} \quad (2.23)$$

of $\mathbf{E}_M(F, \mathfrak{h})$ with Λ_M defined by (2.22) and $y_\ell = (\zeta_1, \dots, \zeta_{\ell-1}, \zeta_{\ell+1}, \dots, \zeta_d)$.

Proof. The proof is based on the multiple use of (2.13) and the triangle inequality combined with the estimation involving the Lebesgue constant (cf. [13, Prop. 4.3]). \blacksquare

In FEM/BEM applications we often deal with functions $G(x)$ defined in a hypercube in \mathbb{R}^d . Specifically, we consider a function $G : (0, 1]^d \rightarrow \mathbb{R}$ which is holomorphic in each variable $x_\ell \in D_\phi(\delta) \supset (0, 1)$, $1 \leq \ell \leq d - 1$, but possibly with a singularity at the endpoint $x_\ell = 0$ of $(0, 1]$. In this case the polynomial interpolation is no longer efficient, however, the Sinc interpolation method can be applied successfully. Given $\alpha \geq 0$, we introduce a possibly modified function $F : \mathbb{R}^d \rightarrow \mathbb{R}$ by

$$F(\zeta_1, \dots, \zeta_d) = \left\{ \prod_{\ell=1}^{d-1} \phi^\alpha(\zeta_\ell) \right\} G(\phi(\zeta_1), \dots, \phi(\zeta_d)) \quad (\phi \text{ from (2.16)}).$$

Next we prove the counterpart of Corollary 2.4 for the error of the multi-variate Sinc interpolation. We define the univariate function $G_\ell(\cdot, y_\ell) : I_\ell \rightarrow \mathbb{R}$ with $I_\ell = (0, 1]$, analogously to the previous construction. Similarly, the function $F(\zeta)$ gives rise to the partially evaluated univariate function $F_\ell(\zeta_\ell, y_\ell)$.

Corollary 2.6 For each $\ell = 1, \dots, d-1$, we assume that for any fixed $y_\ell \in Y_\ell$ the functions $G_\ell(\cdot, y_\ell) : I_\ell \rightarrow \mathbb{R}$ together with their transformed counterparts $F_\ell(\zeta_\ell, y_\ell)$ satisfy the following conditions:

(a) $G_\ell(\cdot, y_\ell)$ is holomorphic on $D_\phi(\delta)$ (cf. (2.17)), and $N(F_\ell, D_\delta) < \infty$ uniformly in $y_\ell \in Y_\ell$;

(b) $F_\ell(\cdot, y_\ell)$ satisfies (2.10) with $a = 1$ and with certain C, b for all $y_\ell \in Y_\ell$.

Then, for all $y_\ell \in Y_\ell$, the optimal choice $\mathfrak{h} := \frac{\log M}{M}$ of the step size yields the pointwise error estimate

$$|G(x) - G_M(x)| \leq \prod_{\ell=1}^{d-1} x_\ell^{-\alpha} |\mathbf{E}_M(F, \mathfrak{h})(\phi^{-1}(x))| \quad (x \in (0, 1]^d = \phi(\mathbb{R}^d)), \quad (2.24)$$

where $\mathbf{E}_M(F, \mathfrak{h})$ is bounded by (2.23) and the corresponding interpolant G_M is given by

$$G_M(x) := \sum_{k_1, k_2, \dots, k_{d-1} = -M}^M G(\phi(k_1 \mathfrak{h}), \dots, \phi(k_{d-1} \mathfrak{h}), x_d) \prod_{\ell=1}^{d-1} \phi^\alpha(k_\ell \mathfrak{h}) \cdot x_\ell^{-\alpha} S_{k_\ell, \mathfrak{h}}(\phi^{-1}(x_\ell)) \approx G(x). \quad (2.25)$$

Proof. Conditions (a), (b) ensure that the corresponding requirements in Proposition 2.5 applied to $F_\ell(\cdot, y_\ell)$ are valid. Then (2.24) is a direct consequence of (2.23). The second assertion holds by definition. ■

The respective Kronecker rank is $r = (2M + 1)^{d-1}$, where M is related to the resulting error ε by $M = \mathcal{O}(\delta^{-1} |\log \varepsilon| \cdot \log |\log \varepsilon|)$. In BEM applications we typically have $\delta = \frac{\pi}{|\log h|}$, where h is the element size (see example in Section 7.5).

3 On Best Approximation by Exponential Sums

In Section 4 we apply the Sinc quadrature¹ to the integral $\frac{1}{\rho} = \int_0^\infty e^{-\rho\xi} d\xi$ and in Section 5 to the integral $\frac{1}{\rho} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^\infty e^{-\rho^2 t^2} dt$ to obtain an exponentially convergent sum of exponentials approximating the inverse function $\frac{1}{\rho}$. Instead, one can directly determine the best approximation of a function with respect to a

certain norm by exponential sums $\sum_{\nu=1}^n \omega_\nu e^{-t_\nu x}$ or $\sum_{\nu=1}^n \omega_\nu e^{-t_\nu x^2}$, where $\omega_\nu, t_\nu \in \mathbb{R}$ are to be chosen optimally.

For special examples we will compare the best approximations with the Sinc quadrature results.

We recall some facts from the approximation theory by exponential sums (cf. [2]). The existence result is based on the fundamental *Big Bernstein Theorem*: If f is completely monotone for $x \geq 0$, i.e.,

$$(-1)^n f^{(n)}(x) \geq 0 \quad \text{for all } n \geq 0, x \geq 0,$$

then it is the restriction of the Laplace transform of a measure to the half-axis:

$$f(z) = \int_{\mathbb{R}_+} e^{-tz} d\mu(t).$$

For $n \geq 1$, consider the set E_n^0 of exponential sums and the extended set E_n :

$$E_n^0 := \left\{ u = \sum_{\nu=1}^n \omega_\nu e^{-t_\nu x} : \omega_\nu, t_\nu \in \mathbb{R} \right\},$$

$$E_n := \left\{ u = \sum_{\nu=1}^\ell p_\nu(x) e^{-t_\nu x} : t_\nu \in \mathbb{R}, p_\nu \text{ polynomials with } \sum_{\nu=1}^\ell (1 + \text{degree}(p_\nu)) \leq n \right\}.$$

Now one can address the problem of finding the best approximation to f over the set E_n characterised by the best approximation error $d(f, E_n) := \inf_{v \in E_n} \|f - v\|_\infty$.

We recall the complete elliptic integral of the first kind with modulus κ ,

$$\mathbf{K}(\kappa) = \int_0^1 \frac{dt}{\sqrt{(1-t^2)(1-\kappa^2 t^2)}} \quad (0 < \kappa < 1)$$

(cf. [22, §1.14.19.1]), and define $\mathbf{K}'(\kappa) := \mathbf{K}(\kappa')$ by $\kappa^2 + (\kappa')^2 = 1$. The following theorem is presented in [2].

¹Generalised Gaussian quadratures for certain improper integrals were described in [21].

Theorem 3.1 Assume that f is completely monotone and analytic for $\Re z > 0$, and let $0 < a < b$. Then² for the uniform approximation on the interval $[a, b]$,

$$\lim_{n \rightarrow \infty} d(f, E_n)^{1/n} \leq \frac{1}{\omega^2}, \quad \text{where } \omega = \exp \frac{\pi \mathbf{K}(\kappa)}{\mathbf{K}'(\kappa)} \quad \text{with } \kappa = \frac{a}{b}.$$

In the case discussed below, we have $\kappa = 1/R$ for possibly large R . Applying the asymptotics

$$\begin{aligned} \mathbf{K}(\kappa') &= \ln \frac{4}{\kappa} + C_1 \kappa + \dots & \text{for } \kappa' \rightarrow 1, \\ \mathbf{K}(\kappa) &= \frac{\pi}{2} \left\{ 1 + \frac{1}{4} \kappa^2 + C_1 \kappa^4 + \dots \right\} & \text{for } \kappa \rightarrow 0, \end{aligned}$$

of the complete elliptic integrals (cf. [8]), we obtain

$$\frac{1}{\omega^2} = \exp \left(-\frac{2\pi \mathbf{K}(\kappa)}{\mathbf{K}(\kappa')} \right) \approx \exp \left(-\frac{\pi^2}{\ln(4R)} \right) \approx 1 - \frac{\pi^2}{\ln(4R)}.$$

The latter expression indicates that the number n of different terms to achieve a tolerance ε is asymptotically

$$n \approx \frac{|\log \varepsilon|}{|\log \omega^{-2}|} \approx \frac{|\log \varepsilon| \ln(4R)}{\pi^2}.$$

This result shows the same asymptotical convergence in n as the corresponding bounds in the later Lemmata 4.3, 5.2.

The best approximation to $1/\rho^\mu$ in the interval $[1, R]$ with respect to a weighted L^2 -norm is reduced to the minimisation of an explicitly given differentiable functional. Given $R > 1$, $\mu > 0$, $N \geq 1$, find the $2N$ real parameters $\alpha_1, \omega_1, \dots, \alpha_N, \omega_N \in \mathbb{R}$, such that

$$F_\mu(R; \alpha_1, \omega_1, \dots, \alpha_N, \omega_N) := \int_1^R W(x) \left(\frac{1}{x^\mu} - \sum_{i=1}^N \omega_i e^{-\alpha_i x} \right)^2 dx = \min. \quad (3.1)$$

In the important particular case of $\mu = 1$ and $W(x) = 1$, the integral (3.1) can be calculated in closed form³:

$$\begin{aligned} F_1(R; \alpha_1, \omega_1, \dots, \alpha_N, \omega_N) &= 1 - \frac{1}{R} - 2 \sum_{i=1}^N \omega_i [\text{Ei}(-\alpha_i) - \text{Ei}(-\alpha_i R)] \\ &+ \frac{1}{2} \sum_{i=1}^N \frac{\omega_i^2}{\alpha_i} [e^{-2\alpha_i} - e^{-2\alpha_i R}] + 2 \sum_{1 \leq i < j \leq N} \frac{\omega_i \omega_j}{\alpha_i + \alpha_j} [e^{-(\alpha_i + \alpha_j)} - e^{-(\alpha_i + \alpha_j) R}] \end{aligned}$$

with the integral exponential function $\text{Ei}(x) = \int_{-\infty}^x \frac{e^t}{t} dt$ (cf. [22, p. 122]). In the special case $R = \infty$, the expression for $F_1(\infty; \dots)$ even simplifies. Gradient or Newton type methods with a proper choice of the initial guess can be used to obtain the minimiser of F_1 .

Optimisation with respect to the maximum norm leads to the nonlinear minimisation problem $\inf_{v \in E_n^0} \|f - v\|_{L^\infty[1, R]}$ involving $2n$ parameters $\{\omega_\nu, t_\nu\}_{\nu=1}^n$. The numerical algorithm follows the Remez algorithm (see [22, §7.5.2]). For our particular application with $f(x) = \frac{1}{x}$ we have the same asymptotical dependence $n = n(\varepsilon, R)$ as in the later Lemmata 4.3 and 5.2, however, the numerical results indicate a noticeable improvement compared with the quadrature method (cf. Lemma 4.3) at least for small numbers $n \leq 15$. Numerical results for the best approximation of $\frac{1}{x}$ by sums of exponentials can be found in [2] and [3]; a full list of numerical data is presented in www.mis.mpg.de/scicomp/EXP_SUM/1_x/tabelle.

4 Integral $\int_0^\infty e^{-\rho t} dt$ and Applications

We consider the Laplace integral transform

$$\frac{1}{\rho} = \int_0^\infty e^{-\rho \xi} d\xi \quad (\rho > 0), \quad (4.1)$$

²The same result holds for E_n^0 , but the best approximation may belong to the closure E_n of E_n^0 .

³In the general case, the integral (3.1) may be approximated by certain quadrature.

with the integrand $f(\xi) = e^{-\rho\xi}$. We assume that ρ varies in $[R_{\min}, R_{\max}]$, where $R_{\min} > 0$ is required, while $R_{\max} = \infty$ is included. Since R_{\min} can be changed by a simple scaling, in the following we use the choice $R_{\min} = 1$, while R_{\max} is renamed by R .

4.1 Standard Quadrature

The substitution $\xi = \log(1 + e^u)$ results into

$$\frac{1}{\rho} = \int_{\mathbb{R}} \frac{e^{-\rho \log(1+e^u)}}{1+e^{-u}} du = \int_{\mathbb{R}} f_1(u) du, \quad f_1(u) := \frac{e^{-\rho \log(1+e^u)}}{1+e^{-u}} \quad (\rho \geq 1). \quad (4.2)$$

This strange looking substitution is chosen to compensate for the unsymmetric behaviour of $e^{-\rho\xi}$. The new integrand f_1 is exponentially decaying for $u \rightarrow \infty$ as well as for $u \rightarrow -\infty$.

For the integral (4.2) we are able to apply the Sinc quadrature.

Lemma 4.1 *Let $\delta < \pi/2$. Then the function from (4.2) satisfies $f_1 \in H^1(D_\delta)$ with a uniform bound $N(f, D_\delta) < \infty$ for all $\rho \geq 1$. In particular, the behaviour is*

$$|f_1(u)| \leq e^{-\rho \Re u} \text{ for } \Re u \geq 0, \quad |f_1(u)| \leq e^{-|\Re u|} \text{ for } \Re u \leq 0 \quad (u \in D_\delta).$$

Under the condition $\rho \geq 1$, (2.5) holds with $C = b = 1$ and the choice $\mathfrak{h} = \sqrt{2\pi\delta/M}$ yields the quadrature result $T_M(f_1, \mathfrak{h})$ with the error estimate (2.8) uniformly for all $\rho \geq 1$.

Proof. a) The zeros of $1 + e^u$ are $\pm ik\pi$ ($k \in \mathbb{Z}_{\text{odd}}$) and therefore outside of D_δ . Hence, $f_1(u)$ is analytic in D_δ .

b) For $u = \xi + i\eta \in D_\delta$ we claim that $\Re \log(1 + e^u) \geq \max(0, \xi)$. For a proof we use

$$\Re \log(1 + e^u) = \frac{1}{2} \log(|1 + e^u|^2) = \frac{1}{2} \log(1 + 2e^\xi \cos(\eta) + e^{2\xi}) \geq \frac{1}{2} \log(e^{2\xi}) = \xi$$

in the case of $\xi \geq 0$ and $\frac{1}{2} \log(1 + 2e^\xi \cos(\eta) + e^{2\xi}) \geq \frac{1}{2} \log(1) = 0$ otherwise.

c) Part b) together with $1/|1 + e^{-u}| \leq 1$ proves the inequality $|f_1(u)| \leq e^{-\rho \Re u}$ for $\Re u \geq 0$.

d) For $\Re u \leq 0$ we use $\Re \log(1 + e^u) \geq 0$ (i.e. $|e^{-\rho \log(1+e^u)}| \leq 1$) and $1/|1 + e^{-u}| \leq 1/|e^{-u}| = e^{\Re u} = e^{-|\Re u|}$.

e) If $\rho \geq 1$, the norm $N(f, D_\delta)$ is bounded independently of ρ and hence the error estimate (2.8) is uniform in ρ . \blacksquare

The finite sum $T_M(f_1, \mathfrak{h})$ can be interpreted as an exponentially convergent quadrature for the integral (4.2). Lemma 4.1 ensures that the tolerance ε can be achieved with $M = \mathcal{O}(|\log \varepsilon|^2)$ uniformly with respect to $\rho \in [1, \infty)$.

4.2 Improved Quadrature

In order to apply the improved estimate (2.11), we apply a second substitution $u = \sinh(w)$ and obtain the integral

$$\frac{1}{\rho} = \int_{\mathbb{R}} f_2(w) dw \quad \text{with } f_2(w) = \cosh(w) f_1(\sinh(w)) = \frac{\cosh(w)}{1 + e^{-\sinh(w)}} e^{-\rho \log(1+e^{\sinh(w)})}. \quad (4.3)$$

The decay of f_2 on the real axis is

$$f_2(w) \approx \frac{1}{2} e^{w - \frac{\rho}{2} e^w} \quad \text{as } w \rightarrow \infty, \quad f_2(w) \approx \frac{1}{2} e^{|w| - \frac{1}{2} e^{|w|}} \quad \text{as } w \rightarrow -\infty,$$

corresponding to $C = \frac{1}{2}$, $b = \min\{1, \rho\}/2$, $a = 1$ in (2.10). A particular difficulty is the behaviour of $f_2(w)$ for $w \in D_\delta$ with $\Re w < 0$, since the exponent $-\rho \log(1 + e^{\sinh(w)})$ may become positive. This effect requires the use of a ρ -dependent δ in the next lemma.

Remark 4.2 *We note that the choice of δ does not change the quadrature, but only effects the error bound (see Proposition 2.1 for the choice of δ).*

As usual, we denote $w = x + iy$, $x, y \in \mathbb{R}$. Note that $\sinh(w) = X + iY$ with

$$X = \sinh(x) \cos(y), \quad Y = \cosh(x) \sin(y) \quad \text{for } w \in D_\delta.$$

Given $\delta < \pi/2$, we introduce the constant $x_1 = x_1(\delta) = \operatorname{arsinh}(\frac{1}{\cos \delta}) > 0$. Now set

$$A := \left(1 + \frac{\pi^2}{4} + \log^2(3\rho)\right) / 2, \quad B := \frac{\pi^2}{4} / \left(A + \sqrt{A^2 + \frac{\pi^2}{4}}\right), \quad (4.4)$$

and define

$$\delta(\rho) := \arcsin(\sqrt{B}), \quad x_0(\rho) := -\operatorname{arsinh}\left(\frac{\log(3\rho)}{\cos(\delta(\rho))}\right) = -\mathcal{O}(\log \log(3\rho)). \quad (4.5)$$

Lemma 4.3 *Let $\delta < \pi/2$. Then the following estimates of f_2 from (4.3) in D_δ cover all values of $x = \Re w$:*

$$\begin{aligned} |f_2(w)| &\leq \frac{\cosh(x)}{1 - e^{-X}} \exp(-\rho \log(e^X - 1)) \Big|_{X=\sinh(x) \cos(y)} \lesssim \frac{1}{2} e^{x - \rho \sinh(x) \cos(y)} \\ &\lesssim \frac{1}{2} e^{x - \rho \frac{\cos(\delta)}{2} e^{|x|}} \quad \text{for } w \in D_\delta, \quad x_1 < x \rightarrow +\infty, \end{aligned} \quad (4.6a)$$

$$|f_2(w)| \leq \sqrt{2} \quad \text{for } w \in D_\delta, \quad 0 \leq x \leq x_1(\delta) \text{ and } \delta \leq 0.93 < \pi/2, \quad (4.6b)$$

$$|f_2(w)| \leq \frac{1}{2} e^{x + \sinh(x) \cos(y)} \leq \frac{1}{2} e^{x - \frac{\cos(\delta)}{2} e^{|x|}} \quad \text{for } w \in D_\delta, \quad x_0(\rho) \leq x \leq 0 \quad (4.6c)$$

$$\text{with } 0 > x_0(\rho) = -\mathcal{O}(\log \log(3\rho)) \text{ and } \delta \leq \delta(\rho) = \mathcal{O}\left(\frac{\pi/2}{\log(3\rho)}\right),$$

$$|f_2(w)| \leq \frac{\sqrt{3}}{1 - 3^{-\cos(\delta)/\cos(\delta(\rho))}} \frac{1}{2} e^{-x + \sinh(x) \cos(y)} \leq C e^{|x| - \frac{\cos(\delta)}{2} e^{|x|}} \quad (4.6d)$$

$$\text{for } w \in D_\delta, \quad 0 > x_0(\rho) \geq x \rightarrow -\infty$$

with $x_0(\rho)$ and $\delta(\rho)$ described in (4.5). Hence $f_2 \in H^1(D_\delta)$, while $\delta \in (0, \delta(\rho)]$ for $\rho \geq 1$ leads to the finite norm $N(f_2, D_\delta) \leq \text{const} < \infty$ independent of ρ . If ρ ranges in $[1, R]$, the choice $\delta = \delta(R)$, $a = 1$, $b = 1/2$ in Proposition 2.1 implies the uniform quadrature error estimate

$$|\eta_M(f_2, \mathfrak{h})| \leq C \exp\left(-\frac{2\pi\delta(R)M}{\log(2\pi M)}\right) \lesssim C \exp\left(-\frac{\pi^2 M}{\log(3R) \log(\pi^2 M)}\right). \quad (4.6e)$$

Proof. a) Again, the zeros of $1 + e^{\sinh(w)}$ are outside of D_δ , so that $f_2(u)$ is analytic in D_δ .

b) The assumption $x > x_1$ ensures $X > 1$. The same argument as in Lemma 4.1 shows $\Re \log(1 + e^{X+iY}) = \frac{1}{2} \log(1 + 2e^X \cos(Y) + e^{2X})$. The worst case is $\cos(Y) = -1$ (which happens only for $x \geq x_0(\delta) > 0$) and yields $\Re \log(1 + e^{X+iY}) \geq \log(e^X - 1)$. This proves (4.6a).

c) $x \leq x_1$ implies $\sinh x \leq \frac{1}{\cos \delta}$. From $\cosh(x) = \sqrt{1 + \sinh^2 x}$ one concludes that $Y = \cosh(x) \sin(y) \leq \tan \delta \sqrt{1 + \cos^2 \delta}$. The restriction $\delta \leq 0.93$ guarantees $Y \in (-\pi/2, \pi/2)$ and thus $\Re e^{X+iY} > 0$. As a consequence $\Re(-\rho \log(1 + e^{\sinh(w)})) < 0$ and $|1 + e^{-\sinh(w)}| > 1$ show $|f_2(w)| \leq |\cosh(w)| \leq \sqrt{1 + \cos^{-2} \delta} \leq \sqrt{2}$.

d) By the definition (4.5) we have that⁴ $\cosh(x) \leq \pi / (2 \sin(\delta(\rho)))$ and $|Y| \leq \frac{\pi}{2}$ holds for $x \geq x_0(\rho)$. This ensures $\Re(-\rho \log(1 + e^{\sinh(w)})) < 0$ and therefore

$$|f_2(w)| \leq \left| \frac{\cosh(w)}{1 + e^{-\sinh(w)}} \right| \leq \frac{e^x}{2(1 + e^{-X})} \leq \frac{1}{2} e^{x + \sinh(x) \cos(y)} \leq \frac{1}{2} e^{x + \sinh(x) \cos(\delta)}.$$

e) For $x \leq x_0(\rho)$ we have $X \leq -\frac{\log(3\rho)}{\cos(\delta(\rho))} \cos y \leq -\log(3\rho)$, so that as in Part b)

$$\Re\left(-\rho \log(1 + e^{\sinh(w)})\right) = -\frac{\rho}{2} \log(1 + 2e^X \cos(Y) + e^{2X}) \leq -\frac{\rho}{2} \log(1 - 2e^X) \leq -\frac{\rho}{2} \log(1 - \frac{2}{3\rho}).$$

⁴With $x_0 = -\operatorname{arsinh}\left(\frac{\log(3\rho)}{\cos(\delta)}\right)$ it follows that $\cosh(x_0) = \sqrt{1 + \sinh^2(x_0)} = \sqrt{1 + \left(\frac{\log(3\rho)}{\cos(\delta)}\right)^2}$. Then the condition $|Y| = |\cosh(x_0) \sin(\delta)| \leq \frac{\pi}{2}$ is equivalent to $\sin^2(\delta) + \tan^2(\delta) \log^2(3\rho) \leq \frac{\pi^2}{4}$. Due to $\tan^2(\delta) = \frac{\sin^2(\delta)}{1 - \sin^2(\delta)}$, we obtain a quadratic equation in $\sin^2(\delta)$, whose solution is given by B from (4.4).

The function $-\frac{\rho}{2} \log(1 - \frac{2}{3\rho})$ decreases with $\rho \geq 1$ leading to $-\frac{\rho}{2} \log(1 - \frac{2}{3\rho}) \leq \frac{\log 3}{2}$ and the bound $\exp(\frac{\log 3}{2}) = \sqrt{3}$ in (4.6d). Together with $1/|1 + e^{-\sinh(w)}| \leq 1/|1 - e^{-X}| = e^X/(1 - e^{-X}) \leq e^X/(1 - e^{-\sinh(x_0(\rho)) \cos(\delta)}) = e^X/(1 - e^{-\frac{\log(3\rho)}{\cos(\delta(\rho))} \cos(\delta)}) = e^X/(1 - 3^{-\cos(\delta)/\cos(\delta(\rho))})$ and $e^X = e^{\sinh(x) \cos(\delta)}$ we obtain (4.6d). ■

Lemma 4.3 ensures that the tolerance ε can be achieved with $M = \mathcal{O}(\log R |\log \varepsilon|)$ uniformly in $\rho \in [1, R]$.

4.3 Numerics

In the numerical example below, we apply the quadrature to f_2 using the simplified choice $\mathfrak{h} = C_0 \frac{\log M}{M}$. All computations in this paper were performed with single precision arithmetic in MATLAB 5.3(R11).

Figures 4.1 and 4.2 (semi-logarithmic scale) illustrate the exponential convergence in the intervals $\rho \in [1, 1000]$ and $\rho \in [1, 18000]$, respectively. The numerical results indicate an almost linear dependence of the quadrature error on ρ , i.e., instead of the slower exponential factor in $\exp(-\frac{\pi^2}{\log(3\rho)} M / \log(\frac{\pi^2 M}{\log(3\rho)}))$ predicted by (4.6e), we observe the behaviour $\mathcal{O}(\rho e^{-cM}) = \mathcal{O}(e^{-cM + \log \rho})$. If this would be true, we obtain a desired error bound ε by $M = \mathcal{O}(\log \frac{1}{\varepsilon} + \log \rho)$.

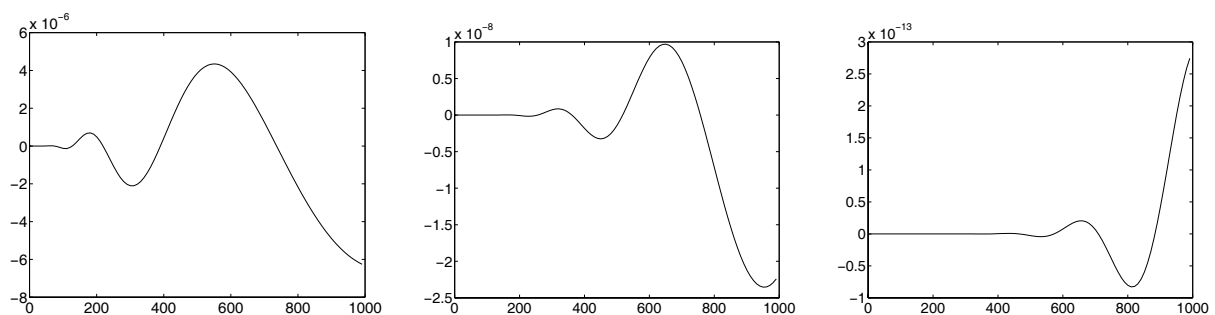


Figure 4.1: The absolute quadrature error for (4.3) for $1 \leq \rho \leq 10^3$ with $M = 16$ (left), $M = 32$ (middle), $M = 64$ (right).

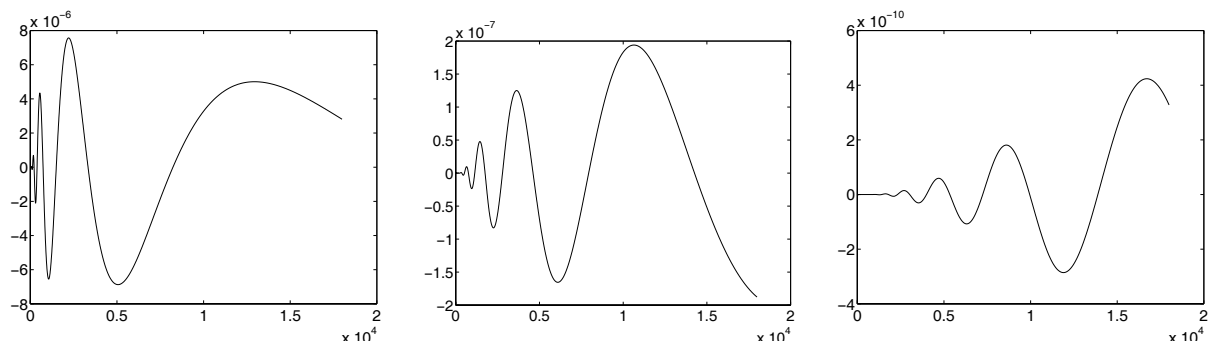


Figure 4.2: The absolute quadrature error for (4.3) for $1 \leq r \leq 18000$ with $M = 16$ (left), $M = 32$ (middle), $M = 64$ (right).

Both the standard and the modified quadrature (cf. Lemma 4.3) can be applied to represent inverse matrices with spectrum in $[1, R]$. In the next examples, we present the error $\|x - A_{(r)}^{-1} Ax\|_\infty$ of different quadratures approximating the inverse of the finite difference Laplacian $A = (-\Delta_h)^{-1}$ in \mathbb{R}^d , where $x \in \mathbb{R}^d$ is chosen as a random tensor-product vector (there is the intrinsic difficulty to calculate a multi-dimensional matrix-norm). Since for all fifty six cases listed in tables below the independent random arrays have been used, we consider the corresponding results as rather convincing. The first table represents the convergence of the order $e^{-c\sqrt{M}}$ of the standard quadrature for (4.1).

standard approximation to $(-\Delta_h)^{-1}$ in $[0, 1]^d$ with $N = n^d$, $n = 128$							
M	4	9	16	25	36	49	64
$d = 3$	5.0_{10-2}	2.0_{10-3}	1.4_{10-4}	1.2_{10-4}	1.7_{10-6}	2.4_{10-8}	1.9_{10-9}
$d = 6$	3.1_{10-3}	5.0_{10-5}	5.3_{10-6}	9.5_{10-7}	5.3_{10-8}	7.7_{10-10}	2.9_{10-12}
$d = 9$	6.7_{10-5}	2.3_{10-7}	1.0_{10-6}	1.0_{10-6}	1.6_{10-9}	3.1_{10-10}	3.1_{10-12}
$d = 12$	2.4_{10-6}	3.2_{10-6}	7.6_{10-8}	7.5_{10-10}	5.7_{10-11}	2.9_{10-13}	6.2_{10-14}

The next table gives the error for the quadrature (4.1) of the order $e^{-cM/\log[\text{cond}(A)]}$. We observe that the latter approximation shows faster exponential convergence for larger M , while the first version is more preferable for smaller M .

improved approximation to $(-\Delta_h)^{-1}$ in $[0, 1]^d$ with $N = n^d$, $n = 128$							
M	4	9	16	25	36	49	64
$d = 3$	2.4_{10-2}	3.8_{10-2}	5.6_{10-2}	9.9_{10-5}	2.6_{10-6}	8.2_{10-10}	7.0_{10-12}
$d = 6$	1.9_{10-2}	1.5_{10-3}	3.7_{10-4}	7.7_{10-7}	4.5_{10-9}	8.2_{10-12}	1.1_{10-14}
$d = 9$	3.0_{10-3}	3.0_{10-3}	1.0_{10-5}	1.6_{10-7}	1.0_{10-9}	1.4_{10-12}	1.7_{10-15}
$d = 12$	3.0_{10-7}	3.9_{10-5}	1.0_{10-8}	7.8_{10-9}	1.8_{10-10}	5.0_{10-13}	5.6_{10-16}

The last table shows that the approximation error depends only weakly on n , confirming the theoretical predictions.

Approximation to $(-\Delta_h)^{-1}$ in $[0, 1]^d$ with $d = 3$, $M = 25$						
n	4	8	16	32	64	128
ε	2.5_{10-8}	7.7_{10-8}	4.2_{10-8}	5.7_{10-7}	8.5_{10-6}	3.5_{10-6}

5 Integral $\int_{-\infty}^{\infty} e^{-\rho^2 t^2} dt$

The integrand of

$$\frac{1}{\rho} = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} e^{-\rho^2 t^2} dt \quad (5.1)$$

shows a fast decay if ρ is not too small. However, the results of §2.3 do not yield uniform error bounds with respect to $\rho \geq 1$. The reason is that $t = x + i\delta \in D_\delta$ results in $|e^{-\rho^2 t^2}| = \exp(-\rho^2(x^2 - \delta^2))$. For $-\delta \leq x \leq \delta$, the exponent is positive and therefore $N(f, D_\delta) \approx \mathcal{O}(e^{\rho^2})$ circumvents reasonable error estimates.

The same difficulty arises when the substitution $t = \sinh(w)$ is used to get the twice exponential decay of the integrand:

$$\frac{1}{\rho} = \int_{-\infty}^{\infty} f_3(w) dw \quad \text{with } f_3(w) = \cosh(w) \exp(-\rho^2 \sinh^2(w)). \quad (5.2)$$

Lemma 5.1 *For each $\rho > 0$, the symmetric $(M + 1)$ -point quadrature for the integral (5.2) converges exponentially with constants C , s in (2.11) depending on ρ .*

Proof. Clearly, for each $\rho > 0$, the function $f_3(w)$ defined above satisfies all the conditions in Proposition 2.1. Thus, we choose $\mathfrak{h} = C_0 \frac{\log M}{M}$ for some C_0 and obtain exponential convergence as indicated in (2.11), where the constants C and s depend on the parameter ρ . ■

We conclude that the symmetric quadrature for the integral (5.2) is acceptable only in an interval $\rho \in I_{ref} = [R_{\min}, R_{\max}]$ with some fixed $R_{\min} \in (0, 1)$ and $R_{\max} > 1$ of order $\mathcal{O}(1)$ (see numerical results below). Hence, for a larger range of the parameter $\rho \in [R_1, R_2]$ we have to split $[R_1, R_2]$ into smaller subintervals and by proper re-scaling reduce each to the approximation in $I_{ref} = [R_{\min}, R_{\max}]$. In general, we need p different intervals, when $R_2/R_1 \approx Q^p$ with $Q = R_{\max}/R_{\min}$.

The following example illustrates the quadrature applied to f_3 . Figure 5.1 shows that stable convergence holds for the range $[0.2, 10]$ of ρ . However, for a fixed value ρ (considered as a constant), the quadrature applies and yields an accuracy ε with $M = \mathcal{O}(\log^2 \frac{1}{\varepsilon})$ (case of (5.1)) or $M = \mathcal{O}(\log \frac{1}{\varepsilon} \cdot \log \log \frac{1}{\varepsilon})$ (case of (5.2)).

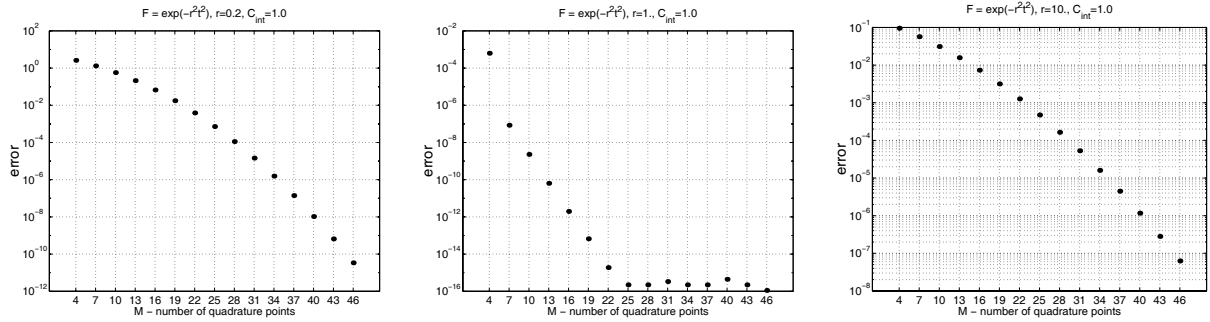


Figure 5.1: Approximation to the integral (5.1) with $\rho \in \{0.2, 1, 10\}$, $\mathfrak{h} = \frac{\log M}{M}$

To obtain robustness with respect to the parameter ρ , we propose another, non-symmetric quadrature. For this purpose we rewrite the integral (5.1) as $\frac{1}{\rho} = \frac{2}{\sqrt{\pi}} \int_0^\infty e^{-\rho^2 t^2} dt$ and then, similar to the previous section, substitute $t = \log(1 + e^u)$ and $u = \sinh(w)$:

$$\frac{1}{\rho} = \int_{\mathbb{R}} f(w) dw \quad \text{with} \quad f(w) := \cosh(w) F(\sinh(w)), \quad F(u) := \frac{2}{\sqrt{\pi}} \frac{e^{-\rho^2 \log^2(1+e^u)}}{1+e^{-u}}. \quad (5.3)$$

Lemma 5.2 *Let $\delta < \pi/2$. Then for the function f from (5.3) we have $f \in H^1(D_\delta)$, and, in addition, the condition (2.10) is satisfied with $a = 1$. For $\rho \geq 1$, the improved $(2M + 1)$ -point quadrature (cf. Proposition 2.1) with the choice $\delta(\rho) = \frac{\pi}{C + \log(\rho)}$ allows the error bound*

$$|\eta_M(f, \mathfrak{h})| \leq C_1 \exp\left(-\frac{\pi^2 M}{(C + \log(\rho)) \log M}\right). \quad (5.4)$$

Proof. It is easy to check that f is holomorphic in D_δ and $N(f, D_\delta) < \infty$ uniformly in ρ . The further analysis is similar to that in Lemma 4.3. \blacksquare

Note that the quadrature error analysis in the more general case $f(\rho) = 1/\rho^\mu$, $\mu > 0$, can be found in [17].

Numerical examples for this quadrature with values $\rho \in [1, R]$, $R \leq 5000$, are presented in Figure 5.2. Again, we observe almost linear error growth in ρ . Similar results are observed in the case $R > 5000$.

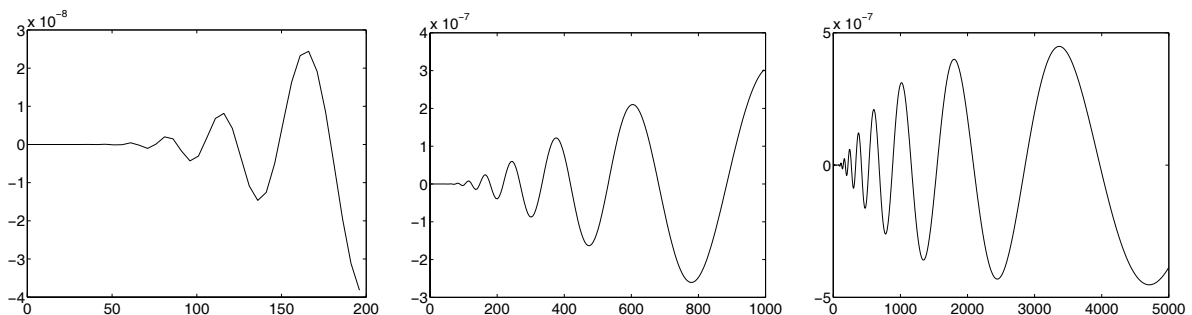


Figure 5.2: The absolute quadrature error for $M = 64$ with $R = 200$ (left), $R = 1000$ (middle), $R = 5000$ (right).

6 Gaussian Charge Distribution

In some cases the precise scaling of the argument, $1 \leq \rho \leq R$, might not be possible as in the following example.

The energy of the interaction between two spherical Gaussian distributions of unit charges centred at $P, P' \in \mathbb{R}^3$ is given by

$$V_{pp'} := \int_{\mathbb{R}^3} \int_{\mathbb{R}^3} \frac{\rho_p(\mathbf{x})\rho_{p'}(\mathbf{y})}{\|\mathbf{x} - \mathbf{y}\|} d\mathbf{x} d\mathbf{y} \quad \text{with } \rho_q(\mathbf{z}) := \left(\frac{q}{\pi}\right)^{3/2} \exp(-q\|\mathbf{z} - P\|^2)$$

(cf. [20]), where $p, p' \in \mathbb{R}$ and $\mathbf{x}, \mathbf{y} \in \mathbb{R}^3$. In fact, the supports of the two Gaussian “basis functions” $\rho_p, \rho_{p'}$ always have an overlap. Therefore, we are going to compare the accuracy of our quadrature from the previous section with that one derived for the explicit expression obtained by analytic spatial integration (often, this integration can be performed only numerically).

The exact integration using the incomplete gamma function $F_0(x) = \int_0^1 e^{-xt^2} dt \equiv \sqrt{\frac{\pi}{4x}} \operatorname{erf}(\sqrt{x})$, leads to

$$V_{pp'} = \sqrt{\frac{4\alpha}{\pi}} F_0\left(\alpha\|P - P'\|^2\right), \quad \alpha = \frac{pp'}{p + p'}.$$

In our example we choose $\alpha = 1$. We use the integral representation on $[0, \infty)$,

$$F_0(x) = \int_0^\infty \exp\left(-x\frac{u^2}{1+u^2}\right) \frac{du}{(1+u^2)^{3/2}} \equiv \int_0^\infty f(u)du, \quad (6.1)$$

and derive the standard quadrature (setting $h = \pi/\sqrt{M}$)

$$F_0(x) \approx h \sum_{k=-M}^M c_k f(u_k), \quad c_k = u_k = e^{kh},$$

which converges as $\mathcal{O}(\exp(-s\sqrt{M}))$. Figure 6.1 shows numerical results for this quadrature with different $M = 25, 64, 121$ and for $x \in [0, R]$, $R = 100$. This example confirms that the exponential convergence is robust in R . Another important observation is that the error bound remains practically the same as that for the integral (5.1) (see Fig. 5.2). This numerical result shows that our exponentially convergent quadrature can be applied to compute accurately the integral $V_{pp'} = \sqrt{\frac{4\alpha}{\pi}} F_0(\alpha\|P - P'\|^2)$ in the wide range of the physical parameter $x = \|P - P'\|^2$.

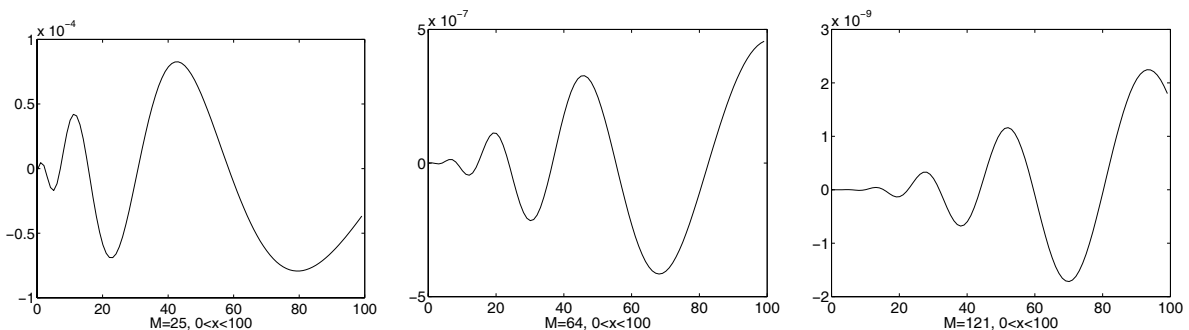


Figure 6.1: The absolute quadrature error for the integrand (6.1) with $M = 25$ (left), $M = 64$ (middle), $M = 121$ (right).

7 Separable Approximation of Multi-Variate Functions

As a by-product, the Sinc quadrature applied to the integrals (4.3) and (5.2) provides a separable approximation to the multi-variate functions

$$\frac{1}{x_1 + \dots + x_d} \quad \text{and} \quad \frac{1}{\sqrt{x_1^2 + \dots + x_d^2}} \quad (x_i > 0, i = 1, \dots, d).$$

In the case of $\frac{1}{x_1+\dots+x_d}$, Lemma 4.3 shows that the separation rank $k = 2M + 1$ depends only linear-logarithmically on both the tolerance $\varepsilon > 0$ and the upper bound R of $\rho = x_1 + \dots + x_d$. In the case of $1/\sqrt{x_1^2 + \dots + x_d^2}$, the dependence on ε and $\rho = \sqrt{x_1^2 + \dots + x_d^2}$ is similar, hence in both cases there is *no dependence on the dimension d* .

In the first case of $\frac{1}{x_1+\dots+x_d}$, the estimate (4.6e) implies that an approximation of accuracy ε is obtainable with

$$M \leq \mathcal{O}\left(\log\left(\frac{1}{\varepsilon}\right) \cdot \log R\right), \quad (7.1)$$

provided that $1 \leq x_1 + \dots + x_d \leq R$, which can be achieved by a proper scaling. The numerical results even support the better estimate $M \leq \mathcal{O}\left(\log\left(\frac{1}{\varepsilon}\right) + \log R\right)$ (see Figures 4.1, 4.2). In the second case of $1/\sqrt{x_1^2 + \dots + x_d^2}$, we apply (5.4) and again obtain the bound (7.1), while our numerical results manifest a rather stable behaviour of the quadrature error with respect to R (see Figure 5.2).

7.1 Example: Newton Potential

Our separable representation to the function $\rho = 1/\sqrt{x_1^2 + \dots + x_d^2}$ directly results in a low Kronecker rank tensor-product approximation (cf. [15]) to the classical Newton potential $(\mathcal{A}u)(x) := \int_{\Omega} \frac{u(y)}{|x-y|} dy$ defined by the kernel function

$$\frac{1}{|x-y|} = \frac{1}{\sqrt{(x_1-y_1)^2 + \dots + (x_d-y_d)^2}} \quad (x, y \in \mathbb{R}^d).$$

Indeed, with the Kronecker rank $r = 2M + 1$, where M satisfies (7.1), we readily obtain the separable approximation of accuracy ε ,

$$\frac{1}{|x-y|} \approx \sum_{k=1}^r C_k f_k^1(|x_1-y_1|) \cdots f_k^d(|x_d-y_d|),$$

provided that $1 \leq |x-y| \leq R$. Note that the Kronecker rank r does not depend on d . In FEM/BEM applications by low order elements, one has $R = \mathcal{O}(h^{-1})$ (after a proper scaling), where h is the mesh parameter.

7.2 Example: $\log(x+y)$

In boundary element methods (BEM), one is interested in a low separation rank representation of the kernel function $s(x, y) = \log(x+y)$, $x \in [0, 1]$, $y \in [h, 1]$ with some small mesh-size parameter $h > 0$ (cf. [14, 15]). A representation like

$$\frac{1}{x+y} = \sum_{m=1}^k \Phi_m(x) \Psi_m(y) + \delta_k \quad \text{with } |\delta_k| \leq \varepsilon \quad (7.2)$$

can be constructed by means of the quadrature applied to the integral (4.3) with $\rho = x+y$ and $k = 2M + 1$. Let ψ_m be the anti-derivatives of Ψ_m . Integration of (7.2) yields

$$\begin{aligned} \log(x+y) &= \int_{1-x}^y \frac{dt}{x+t} = \int_{1-x}^y \left(\sum_{m=1}^k \Phi_m(x) \Psi_m(t) + \delta_k \right) dt \\ &= \sum_{m=1}^k \Phi_m(x) [\psi_m(y) - \psi_m(1-x)] + S_k = \Phi_0(x) + \sum_{m=1}^k \Phi_m(x) \psi_m(y) + S_k \end{aligned}$$

with $\Phi_0(x) = -\sum_{m=1}^k \Phi_m(x) \psi_m(1-x)$ and $|S_k| = \left| \int_{1-x}^y \delta_k dt \right| \leq \varepsilon$. This resulting representation of $\log(x+y)$ has the separation rank $k+1$ and the same accuracy ε as (7.2).

In the next example we illustrate how to apply Corollary 2.4.

7.3 Example: $1/(x+y)$

Interesting examples like $g(x, y) = \frac{1}{x+y}$ ($x, y > 0$) have a singularity at $x = -y$. In the following, we discuss the choice of δ such that g is holomorphic in the strip $D_\phi(\delta)$ (see §2.5). Solving the equation $\cosh(z) = -1/y$, we find the singularity points $z_m = \pm \operatorname{arcosh}(1/y) + (1 \pm 2m)i\pi$, $m = 0, 1, \dots$. Now, by solving the equation $\sinh(\zeta_m) = z_m$ we find $\zeta_m = \log(z_m + \sqrt{1 + z_m^2})$, $\Im\zeta_m = \arg(z_m + \sqrt{1 + z_m^2})$. Suppose that $y \rightarrow 0$, hence $\min_{m \in \mathbb{N}_0} \{\Im\zeta_m\} \geq C_0\pi / \operatorname{arcosh}(1/y)$ is achieved with $m = 0$, where C_0 does not depend on y (we actually have $C_0 \approx 1$). Taking $m = 0$ and suppressing all symmetric images, we come to the conclusion that $g(\phi(\zeta), y)$ is holomorphic in D_{δ_0} , where $\tan(\delta_0) = C_0\pi / \operatorname{arcosh}(1/y)$ depends on y .

In the following, we fix $y > 0$ and, first, apply Corollary 2.4 with

$$\delta = \delta_0 = \arctan(C_0\pi / \operatorname{arcosh}(1/y)),$$

and next (2.20) to obtain

$$|g(x, y) - g_M(x, y)| \leq C |x|^{-\alpha} \frac{N(f, D_\delta)}{2\pi\delta_0} e^{-\pi\delta_0 M / \log M}. \quad (7.3)$$

In BEM applications we have $x, y \geq h \rightarrow 0$, where $h > 0$ is the mesh parameter, so that $\delta_0 \approx \frac{\pi}{|\log h/2|}$ depends only mildly on h . Then (7.3) leads to

$$|g(x, y) - g_M(x, y)| \leq C |h|^{-\alpha} \frac{N(f, D_\delta) |\log h/2|}{2\pi^2} e^{-\pi^2 M / (|\log h/2| \log M)}. \quad (7.4)$$

Hence, the tolerance ε can be achieved with $M = O(|\log h| |\log \varepsilon|)$ and with the Kronecker rank $r = 2M + 1$.

Note that the error estimate for the function $1/(x+y)$, $x, y \in [1, R]$, can be derived from (7.4) by the substitution $h = 1/R$.

Similarly to the previous example, the Sinc approximation can be applied to functions like $g(x, y) = \log(x+y)$, $g(x, y) = (x^2 + y^2) \log(x+y)$ (biharmonic kernel function) and to $H_0^{(1)}(x+y)$ (2D Helmholtz kernel).

7.4 Example: $\exp(-xy)$

Next, we discuss the function $g(x, y) = \exp(-xy)$, $x \geq 0$, $y \in [1, \lambda_{\max}] \subset [1, \infty)$, which arises in Part II of our paper.

We consider the auxiliary function $f(x, y) = \frac{x}{1+x} \exp(-xy)$, $x \in \mathbb{R}_+$. This function satisfies all the conditions of [18, Example 4.2.11] with $\alpha = \beta = 1$ (see also [7, §2.4.2]), and hence, with the corresponding choice of interpolation points $x_k := \log[e^{k\mathfrak{h}} + \sqrt{1 + e^{2k\mathfrak{h}}}] \in \mathbb{R}_+$, it can be approximated by

$$\sup_{0 < x < \infty} \left| f(x, y) - \sum_{k=-M}^M f(x_k, y) S(k, \mathfrak{h}) (\log\{\sinh(x)\}) \right| \leq CM^{1/2} e^{-cM^{1/2}}$$

with exponential convergence, where $S(k, \mathfrak{h})$ is the k -th Sinc function (cf. (2.3)) and $\mathfrak{h} = C_1/M^{1/2}$. The corresponding error estimate for the function $g(x, y)$ is given by (2.20) with $\alpha = 1$ (cf. [17] for the corresponding numerical examples).

Alternatively, we can apply the integral representation (for $x, y \geq c > 0$)

$$\exp(-2xy) = \frac{x}{\sqrt{\pi}} \int_{\mathbb{R}_+} s^{-3/2} \exp(-x^2/s - sy^2) ds,$$

or, via the substitution $s = e^t$,

$$\exp(-2xy) = \frac{x}{\sqrt{\pi}} \int_{\mathbb{R}} \exp\left(-\frac{t}{2} - x^2 e^{-t} - y^2 e^t\right) dt.$$

Hence, one can approximate $g(x, y) = \exp(-xy)$ directly by an double exponential sum, i.e.,

$$\exp(-xy) \approx \sum_{1 \leq i \leq j \leq r} c_{ij} e^{-b_i x^2} e^{-b_j y^2}, \quad (x, y) \in [0, R]^2,$$

with symmetric coefficient matrix $c_{ij} = c_{ji}$. The corresponding minimisation problem for the L^2 -norm error functional takes the form

$$\text{minimise} \quad \left\| \exp(-xy) - \sum_{1 \leq i \leq j \leq r} c_{ij} e^{-b_i x^2} e^{-b_j y^2} \right\|_{L^2}^2 \quad \text{with respect to } c_{ij}, b_i,$$

which can be solved by the Newton-type methods. The separation rank is r , since $\exp(-xy) \approx \sum_{i=1}^r \Phi_i(x) \Psi_i(y)$ with $\Phi_i(x) = e^{-b_i x^2}$ and $\Psi_i(y) = \sum_{j=1}^r c_{ij} e^{-b_j y^2}$.

Alternatively, the coefficients b_i, b_j can be precomputed by using certain approximations for $\exp(-cy)$ by exponential sums ($c > 0$: lower bound of the variable x). Then the L^2 -orthogonal projection onto $\text{span}\{e^{-b_i x^2} e^{-b_j y^2}\}$ determines the coefficients c_{ij} .

7.5 Example: Helmholtz Kernel in \mathbb{R}^d

We consider the singularity function corresponding to the Helmholtz operator in \mathbb{R}^d , $d \geq 2$. Given $\kappa \in \mathbb{R}$, define the Helmholtz kernel function

$$g(x, y) := \frac{\cos(\kappa|x-y|)}{|x-y|} = \Re e \frac{e^{i\kappa|x-y|}}{|x-y|} \quad \text{for } (x, y) \in [0, 1]^d \times [0, 1]^d$$

in Cartesian coordinates $x = (x_1, \dots, x_d), y = (y_1, \dots, y_d) \in \mathbb{R}^d$. We mention that an analysis of polynomial approximations to the Helmholtz kernel function is presented in [13] in the context of the hierarchical matrix technique with standard admissibility criteria. The Sinc approximation below can be applied in the case of a weakly admissible block (cf. [14]) with respect to the transformed variables ζ_1, \dots, ζ_d .

For $(\zeta_1, \dots, \zeta_d) \in [0, 1]^d$, define

$$G(\zeta_1, \dots, \zeta_d) := g(x, y), \quad \zeta_\ell = |x_\ell - y_\ell|, \quad \ell = 1, \dots, d,$$

which implies

$$G(\zeta_1, \dots, \zeta_d) := \cos\left(\kappa \sqrt{\zeta_1^2 + \dots + \zeta_d^2}\right) / \sqrt{\zeta_1^2 + \dots + \zeta_d^2}.$$

We approximate the modified function

$$F(\zeta_1, \dots, \zeta_d) := (\zeta_1 \cdot \dots \cdot \zeta_{d-1})^{\alpha_0} G(\zeta_1, \dots, \zeta_d), \quad 0 < \alpha_0 < 1,$$

on the domain $\Omega_1 := [0, 1]^{d-1} \times [h, 1]$, where $h > 0$ is a small parameter, which can be associated with the mesh-size.

Now we apply Corollary 2.6 with $\delta = 1/|\log h|$ to construct the approximation $G_M(x)$ via the interpolation of F and obtain

$$\begin{aligned} |G(x) - G_M(x)| &\leq \prod_{\ell=1}^{d-1} x_\ell^{-\alpha_0} |\mathbf{E}_M(F, h)(\phi^{-1}(x))| \\ &\leq Ch^{\alpha_0(1-d)} |\log h| \Lambda_M^{d-1} N_0(F, D_\delta) e^{-\pi M / (|\log h| \log M)} \end{aligned} \quad (7.5)$$

with $\zeta \in (0, 1]^d$, where the corresponding interpolant $G_M(x)$ is given by (2.25).

Note that in this example $N_0(F, D_\delta) = \mathcal{O}(e^\kappa)$, while the Kronecker rank is given by $r = (2M + 1)^{d-1}$. Clearly, for a large parameter κ , the bound (7.5) does not provide a satisfactory complexity.

The intrinsic alternative to the multi-variate Sinc interpolation would be the following two-step method: First, compute the polynomial interpolation to the entire function $\cos(\kappa \sqrt{\zeta_1^2 + \dots + \zeta_d^2})$ with $r = \mathcal{O}((\log R |\log \varepsilon|)^{d-1})$ and then multiply it with the HKT representation to the Newton potential as above. However, in this case the resulting Kronecker rank (obtained as a product of the corresponding ranks for the elementary factors) seems to be larger than for the Sinc interpolation method.

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