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Approximation by exponential sums revisited ☆

Gregory Beylkin *, Lucas Monzón

Department of Applied Mathematics, University of Colorado, Boulder, CO 80309-0526, United States

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ABSTRACT

We revisit the efficient approximation of functions by sums of exponentials or Gaussians in Beylkin and Monzón (2005) [16] to discuss several new results and applications of these approximations. By using the Poisson summation to discretize integral representations of e.g., power functions $r^{-\beta}$, $\beta > 0$, we obtain approximations with uniform relative error on the whole real line. Our approach is applicable to a class of functions and, in particular, yields a separated representation for the function e^{-xy}. As a result, we obtain sharper error estimates and a simpler method to derive trapezoidal-type quadratures valid on finite intervals. We also introduce a new reduction algorithm for the case where our representation has an excessive number of terms with small exponents.

As an application of these new estimates, we simplify and improve previous results on separated representations of operators with radial kernels. For any finite but arbitrary accuracy, we obtain new separated representations of solutions of Laplace's equation satisfying boundary conditions on the half-space or the sphere. These representations inherit a multiresolution structure from the Gaussian approximation leading to fast algorithms for the evaluation of the solutions. In the case of the sphere, our approach provides a foundation for a new multiresolution approach to evaluating and estimating models of gravitational potentials used for satellite orbit computations.

1. Introduction

In this paper we revisit the efficient approximation of functions by sums of exponentials or Gaussians, a problem that has been considered in [16]. As a tool, this type of nonlinear approximations have been instrumental in constructing separated representations of integral operators. In particular, separated representations of non-oscillatory Green's functions using Gaussians found applications in quantum chemistry [7,9,26,27,33,34] and in an approach to solve Schrödinger's equation [13,14]. Additional applications of approximations by sums of exponentials involve evaluation of oscillatory Green's functions in [11,12], nonlinear inversion of band-limited Fourier transform in [17], as well as quadratures for functions band-limited in a disk [10].

In quantum chemistry early examples of nonlinear approximations by Gaussians appeared in [18,30,32] to approximate the wavefunctions and, later, in [28] to approximate the Coulomb potential. Approximation of $1/r$ by sum of exponentials has been also been studied in [35] and [20,21].

As the development of applications lead to a better understanding of the features of these approximations, we decided to revisit this topic to further elaborate on some of them. In particular, we have shown in [16] how to approximate, for any

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* Corresponding author.
E-mail address: beylkin@colorado.edu (G. Beylkin).

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given accuracy $\epsilon > 0$ and distance to the singularity $\delta > 0$, the power functions $r^{-\beta}$, $\beta > 0$, with a linear combination of exponentials,

$$\left| r^{-\beta} - \sum_{m=1}^{M} w_m e^{-p_m r} \right| \leqslant r^{-\beta}\epsilon, \tag{1}$$

for $r \in [\delta, 1]$. As we have pointed out in [16], our standard algorithm to obtain the minimal number of positive weights w_m and positive exponents p_m (see Appendix A.1) is ill-suited in this case due to the rapid growth of the function near zero and the resulting large number of samples necessary to cover the range of interest when δ is very small. On the other hand, using the reduction procedure [16, Section 6], we only need an accurate initial approximation to then minimize the number of terms M in (1) without experiencing the size constraints. Such initial approximation for (1) is based upon using the trapezoidal rule to discretize the integral

$$r^{-\beta} = \frac{1}{\Gamma(\beta)} \int_{-\infty}^{\infty} e^{-re^t + \beta t}\, dt, \tag{2}$$

for $r \in [\delta, 1]$. The trapezoidal rule yields an explicit but suboptimal discretization of (2) as a sum of exponentials. Remarkably, this approximation attains a uniform relative error on the whole range of interest. In [16] we use the Euler–Maclaurin formula to estimate the number of terms in the discretization of (2) as a function of the accuracy and the range of r. Here, in Section 2, we consider a different, simpler way to obtain the initial approximation and estimate its number of terms using Poisson's formula (which, incidentally, implies Euler–Maclaurin formula [5, p. 626]). This leads to a new approach to estimate the error of approximating power functions by linear combinations of exponentials or Gaussians. Our approach is also applicable to other functions of interest. In particular, we develop an approximation of e^{-xy}, $x, y > 0$, as a separated sum of Gaussians in Section 2.2 and provide an example of its application in Section 5.3.

In all of these cases the initial approximations obtained via discretization of integrals are suboptimal and may contain an excessive number of terms, e.g., those terms corresponding to small exponents. To reduce the number of terms, in Section 3 we introduce a simple algorithm based on Prony's method as an alternative to the more general reduction algorithm [16, Section 6].

In Section 4 we simplify and improve previous error estimates for separated representations of operators with radial kernels.

In Section 5 we derive new separated multiresolution representations for Poisson's kernels for the half-space and the sphere. We then describe an application of such representations to modeling gravity potentials (used for satellite orbit computations) and provide a foundation for a new multiresolution approach to evaluating and estimating such models.

2. Quadratures using Poisson's formula

We consider the problem of obtaining a trapezoidal quadrature for an integral over the real line

$$I = \int_{\mathbb{R}} f(t)\, dt, \tag{3}$$

where we assume a sufficient decay of the function f and its Fourier transform

$$\hat{f}(\xi) = \int_{\mathbb{R}} f(t) e^{-2\pi i \xi t}\, dt.$$

By Poisson's summation formula, we have

$$\sum_{n\in\mathbb{Z}} \hat{f}\left(\frac{n}{h}\right) e^{2\pi i t_0 \frac{n}{h}} = h \sum_{n\in\mathbb{Z}} f(t_0 + nh), \tag{4}$$

where $t_0 \in \mathbb{R}$ and $h > 0$ are chosen later. Since $\hat{f}(0) = \int_{\mathbb{R}} f(t)\, dt$,

$$\left| \int_{\mathbb{R}} f(t)\, dt - h \sum_{n\in\mathbb{Z}} f(t_0 + nh) \right| \leqslant \sum_{n\neq 0} \left| \hat{f}\left(\frac{n}{h}\right) \right|. \tag{5}$$

Thus, a fast decay of $\hat{f}$, the Fourier transform of the integrand in (3), allow us to choose the step size h so that (5) achieves the accuracy sought. In this way, the integral (3) may be approximated by an infinite sum of uniformly sampled values of f. We show

Proposition 1. *Let us assume that* (4) *holds. For any* $\epsilon > 0$ *and* $t_0 \in \mathbb{R}$, *we have*

$$\left| \int_{\mathbb{R}} f(t)\,dt - h \sum_{n\in\mathbb{Z}} f(t_0 + nh) \right| \leqslant \epsilon \tag{6}$$

provided that the Fourier transform of f *satisfies*

$$\left|\hat{f}(\xi)\right| \leqslant c_1 e^{-q|\xi|}, \tag{7}$$

for some positive constants c_1, q *and step size* $h \leqslant q/\log(2c_1\epsilon^{-1}+1)$ *or, alternatively,*

$$\left|\hat{f}(\xi)\right| \leqslant \frac{c_2}{|\xi|^q}, \quad \text{for } |\xi| \geqslant R, \tag{8}$$

for some positive constants c_2, R, q *and step size* $h \leqslant \min\{1/R, \epsilon^{1/q}(2c_2\zeta(q))^{-1/q}\}$, *where* $\zeta(q)$ *is the Riemann Zeta function.*

Proof. From (5), it is enough to derive conditions on h so that $\sum_{n\neq 0} |\hat{f}(\frac{n}{h})| \leqslant \epsilon$. Under (7), we have

$$\sum_{n\neq 0}\left|\hat{f}\left(\frac{n}{h}\right)\right| \leqslant 2c_1 \frac{1}{e^{q/h}-1} \leqslant \epsilon$$

if $h \leqslant q/\log(2c_1\epsilon^{-1}+1)$ and, under (8), for $1/h \geqslant R$,

$$\sum_{n\neq 0}\left|\hat{f}\left(\frac{n}{h}\right)\right| \leqslant 2c_2 h^q \sum_{n=1} n^{-q} \leqslant 2c_2 h^q \zeta(q) \leqslant \epsilon$$

if $h \leqslant \epsilon^{1/q}(2c_2\zeta(q))^{-1/q}$. □

Remark 2. Applying Proposition 1 to functions with compact support, we may recover the Euler–Mclaurin formula to estimate the error of the trapezoidal rule. Note that the decay of $\hat{f}$ is related to the smoothness of f. Also, one may recover the Bernoulli numbers B_q, appearing in the Euler–Mclaurin formula, since for positive integer q, the Riemann Zeta function $\zeta(2q)$ may be written in terms of B_{2q}. For details we refer to [5, p. 626].

If the function f in (6) has fast decay, then the infinite sum may be replaced by a finite sum, providing a finite quadrature for the integral (3). In [23] S. Dubuc followed this approach to obtain an approximation of the Gamma function. A similar approach was used in [6, Eq. (2.13)] to obtain estimates for the Unequally Spaced Fast Fourier Transform (USFFT). In this paper, we use Proposition 1 as a starting point to obtain a representation of power functions $r^{-\beta}$, $r, \beta > 0$, in terms of Gaussians or exponentials, as well as to represent the exponential function e^{-xy}, $x, y > 0$, as a separated sum of Gaussians. We also show how the method may be adapted to find approximations to other functions.

2.1. Power functions $r^{-\beta}$

Let us apply Proposition 1 to power functions to obtain their approximations by exponentials. Writing (2) as

$$r^{-\beta} = \int_{-\infty}^{\infty} f(t)\,dt, \tag{9}$$

where

$$f(t) = f_{\beta,r}(t) = \frac{1}{\Gamma(\beta)} e^{-re^t+\beta t}, \tag{10}$$

we compute the Fourier transform of f in (10),

$$\hat{f}(\xi) = \frac{1}{\Gamma(\beta)} \int_{\mathbb{R}} e^{-re^t+\beta t} e^{-2\pi i\xi t}\,dt = \frac{\Gamma(\beta - 2\pi i\xi)}{\Gamma(\beta)} r^{2\pi i\xi-\beta}. \tag{11}$$

We note that f and $\hat{f}$ both have exponential or super exponential decay at $\pm\infty$ and, hence, this particular integral representation of $r^{-\beta}$ is suitable for the Poisson approach described above. Following (5), we need to bound

$$\left|r^{-\beta} - S_\infty(r)\right| \leqslant r^{-\beta} \sum_{n\neq 0} \frac{|\Gamma(\beta + 2\pi i\frac{n}{h})|}{\Gamma(\beta)}, \tag{12}$$

where

$$S_\infty(r) = \frac{h}{\Gamma(\beta)} \sum_{n\in\mathbb{Z}} e^{\beta(t_0+nh)} e^{-e^{t_0+nh} r}. \tag{13}$$

Next we show how to choose $h = h(\epsilon, \beta)$ as to yield

$$\sum_{n\neq 0} \frac{|\Gamma(\beta + 2\pi i \frac{n}{h})|}{\Gamma(\beta)} < \epsilon. \tag{14}$$

Theorem 3. *Given $\beta > 0$ and $0 < \epsilon \leqslant 1$, for any step size h such that*

$$h \leqslant \frac{2\pi}{\log 3 + \beta \log(\cos 1)^{-1} + \log \epsilon^{-1}}, \tag{15}$$

and any $t_0 \in \mathbb{R}$ we have

$$\frac{|r^{-\beta} - S_\infty(r)|}{r^{-\beta}} \leqslant \epsilon, \quad \textit{for all } r > 0, \tag{16}$$

where S_∞ is given in (13).

We note that $S_\infty(r)$ in (16) provides a uniform approximation with respect to r. Therefore, for a given accuracy ϵ and power β, we may first select h and then, for a given range of values r, truncate $S_\infty(r)$ to yield a finite sum approximation in that range. In this regard the approach here differs from our previous derivation in [16] and plays an important role in subsequent estimates.

Proof. As n increases, $|\Gamma(\beta + 2\pi i \frac{n}{h})|$ decays exponentially fast and we may simply compute the largest value of h to satisfy (14). To obtain an analytic estimate of h, we use the integral representation [25, 6.312.5],

$$\Gamma(z) = e^{i\theta z} \int_0^\infty e^{-te^{i\theta}} t^{z-1}\, dt,$$

valid for $\mathrm{Re}(z) > 0$ and $|\theta| < \frac{\pi}{2}$. Therefore, for positive β and y, and $0 < \theta < \frac{\pi}{2}$, we have

$$\left|\Gamma(\beta + iy)\right| \leqslant e^{-\theta y} \int_0^\infty e^{-t\cos\theta} t^{\beta-1}\, dt = \Gamma(\beta)(\cos\theta)^{-\beta} e^{-\theta y},$$

and setting $\theta = 1$ and $y = \frac{2\pi}{h}$, obtain

$$\frac{|\Gamma(\beta + 2\pi i/h)|}{\Gamma(\beta)} \leqslant (\cos 1)^{-\beta} e^{-2\pi/h}.$$

Substituting in (12) yields (15), since we have

$$\frac{|r^{-\beta} - S_\infty(r)|}{r^{-\beta}} \leqslant 2(\cos 1)^{-\beta} \sum_{n\geqslant 1} e^{-2\pi n/h} = \frac{2(\cos 1)^{-\beta}}{e^{2\pi/h} - 1} < \epsilon, \tag{17}$$

provided that

$$\log\bigl(2(\cos 1)^{-\beta}\epsilon^{-1} + 1\bigr) \leqslant \log\bigl(3(\cos 1)^{-\beta}\epsilon^{-1}\bigr) \leqslant 2\pi/h. \qquad \square$$

2.1.1. Approximation by finite sums

Let us truncate the infinite sum $S_\infty(r)$ in (13) to obtain a finite sum $S_F(r)$,

$$S_F(r) = S_F(r; M, N, h) = \frac{h}{\Gamma(\beta)} \sum_{n=M+1}^{N} e^{-re^{t_0+nh} + \beta(t_0+nh)}, \quad r > 0. \tag{18}$$

We estimate the tails of $S_\infty(r)$, i.e. find M, N and h satisfying (15), so that

$$\left|\frac{r^{-\beta} - S_F(r)}{r^{-\beta}}\right| < \epsilon, \quad \text{for } 0 < \delta \leqslant r \leqslant 1. \tag{19}$$

Given (19), we have

Lemma 4. *For all $r > 0$,*

$$S_F(r) < S_\infty(r) < (\epsilon + 1)r^{-\beta}.$$

This estimate shows that our approximation, $S_F(r)$, is effectively bounded by the true function *on the whole positive axis*, a result already used in [12]. In Section 4 we use this lemma to simplify and correct some estimates in [9].

Proof. The first inequality follows since f in (10) is a positive function for all positive r and β. The second inequality follows from (16). □

The number of terms in S_F depends on the parameters β, δ and ϵ, and is described in

Theorem 5. *For any $\beta > 0$, $\delta > 0$, and $1/e \geqslant \epsilon > 0$, there exist a step size h and integers M and N such that*

$$\left|r^{-\beta} - S_F(r; M, N, h)\right| \leqslant r^{-\beta}\epsilon, \quad \text{for all } \delta \leqslant r \leqslant 1, \tag{20}$$

where

$$S_F(r; M, N, h) = \frac{h}{\Gamma(\beta)} \sum_{n=M+1}^{N} e^{\beta hn} e^{-e^{hn} r}. \tag{21}$$

For fixed β, the step size satisfies $h = \mathcal{O}(1/\log \epsilon^{-1})$ and the number of terms in $S_F(r; M, N, h)$ may be estimated as

$$N - M \leqslant \frac{1}{10}\left(2\log\epsilon^{-1} + \log\beta + 2\right)\left(\log\delta^{-1} + \frac{1}{\beta}\log\epsilon^{-1} + \log\log\epsilon^{-1} + \frac{3}{2}\right). \tag{22}$$

Therefore, for fixed power β and accuracy ϵ, we have $N - M = \mathcal{O}(\log\delta^{-1})$, where M is typically negative.

Also, we have

$$\left|r^{-\beta} - S_F(r; M, \infty, h)\right| \leqslant r^{-\beta}\epsilon, \quad \text{for all } 0 < r \leqslant 1. \tag{23}$$

By setting $\beta = \alpha/2$, replacing r by r^2 and δ by δ^2, Theorem 5 may also be interpreted as an approximation of power functions via Gaussians.

Theorem 6. *For any $\alpha > 0$, $\delta > 0$, and $1/e \geqslant \epsilon > 0$, there exist a step size h and integers M and N such that*

$$\left|r^{-\alpha} - G_F(r; M, N, h)\right| \leqslant r^{-\alpha}\epsilon, \quad \text{for all } \delta \leqslant r \leqslant 1, \tag{24}$$

where

$$G_F(r; M, N, h) = \frac{h}{\Gamma(\alpha/2)} \sum_{n=M+1}^{N} e^{\alpha hn/2} e^{-e^{hn} r^2}. \tag{25}$$

For fixed power α and accuracy ϵ, the number of terms is $N - M = \mathcal{O}(\log\delta^{-1})$.

Also, we have

$$\left|r^{-\alpha} - G_F(r; M, \infty, h)\right| \leqslant r^{-\alpha}\epsilon, \quad \text{for all } 0 < r \leqslant 1. \tag{26}$$

Let us outline our approach to prove Theorem 5 and refer to Appendix A.3 for the details. Since for all $r > 0$,

$$\left|\frac{r^{-\beta} - S_F(r)}{r^{-\beta}}\right| \leqslant \left|\frac{r^{-\beta} - S_\infty(r)}{r^{-\beta}}\right| + \left|\frac{S_\infty(r) - S_F(r)}{r^{-\beta}}\right|,$$

we need to estimate these two terms. The first term may be bound using the estimate (16) provided we select the step size h according to (15). To bound the second term, we truncate $S_\infty(r)$ and consider the lower tail

$$\mathcal{T}_M(r) = \frac{r^\beta}{\Gamma(\beta)} h \sum_{n \leqslant M} e^{-re^{t_n} + \beta t_n},$$

and the upper tail

$$\mathcal{T}^N(r) = \frac{r^\beta}{\Gamma(\beta)} h \sum_{n \geqslant N+1} e^{-re^{t_n} + \beta t_n}.$$

By selecting M and N, we bound both tails by ϵ in some target range $r \in [\delta, 1]$. To majorate both tails by an integral, consider again the integrand $f_{\beta,r}(y)$ in (9)–(10) which has a global maximum at $y_0 = \log(r^{-1}\beta)$. Hence, for any M satisfying $t_M \leqslant \log\beta$ the function $f_{\beta,r}(y)$ is decreasing on $(-\infty, t_M)$ for all $r \in (0, 1]$ and we may estimate the lower tail $\mathcal{T}_M(r)$ by the associated integral

$$\mathcal{T}_M(r) \leqslant \frac{r^\beta}{\Gamma(\beta)} \int_{-\infty}^{t_M} e^{-re^y+\beta y}\,dy \leqslant \frac{1}{\Gamma(\beta)} \int_{-\infty}^{t_M} e^{-e^y+\beta y}\,dy \tag{27}$$

$$= \frac{1}{\Gamma(\beta)} \int_0^{e^{t_M}} e^{-s} s^{\beta-1}\,ds = 1 - \frac{\Gamma(\beta, e^{t_M})}{\Gamma(\beta)}, \tag{28}$$

where

$$\Gamma(\beta, x) = \int_x^\infty e^{-s} s^{\beta-1}\,ds$$

is the incomplete Gamma function. We note that t_M does not depend on δ.

Similarly, with N satisfying

$$t_N \geqslant \log\left(\delta^{-1}\beta\right), \tag{29}$$

the corresponding upper tail satisfies

$$\mathcal{T}^N(r) \leqslant \frac{r^\beta}{\Gamma(\beta)} \int_{t_N}^{\infty} e^{-re^y+\beta y}\,dy = \frac{1}{\Gamma(\beta)} \int_{re^{t_N}}^{\infty} e^{-s} s^{\beta-1}\,ds,$$

for all $r \in [\delta, 1]$ and we obtain

$$\mathcal{T}^N(r) \leqslant \frac{\Gamma(\beta, \delta e^{t_N})}{\Gamma(\beta)}. \tag{30}$$

Since

$$\lim_{x\to 0} \frac{\Gamma(\beta, x)}{\Gamma(\beta)} = 1 \quad \text{and} \quad \lim_{x\to\infty} \frac{\Gamma(\beta, x)}{\Gamma(\beta)} = 0,$$

we may achieve any target accuracy ϵ by defining t_* and t^* as solutions of the equations,

$$1 - \frac{\Gamma(\beta, e^{t_*})}{\Gamma(\beta)} = \epsilon, \tag{31}$$

and

$$\frac{\Gamma(\beta, \delta e^{t^\star})}{\Gamma(\beta)} = \epsilon. \tag{32}$$

To establish corresponding integers M_* and N^* in the definition of S_F, we may have to modify slightly t_*, t^*, or h and select t_0, so that both $(t_* - t_0)/h$ and $(t^* - t_0)/h$ are integers. We prove

Lemma 7. *For all $\beta > 0$, $\delta > 0$ and $1/e \geqslant \epsilon > 0$, the solution t_* of* (31) *does not depend on δ and satisfies*

$$t_* \geqslant \frac{\log \epsilon\Gamma(1+\beta)}{\beta} = \frac{1}{\beta}\log\epsilon + \log\Gamma(1+\beta)^{\frac{1}{\beta}}. \tag{33}$$

The solution t^* of (32) *has a weak dependence on ϵ and satisfies*

$$t^* \leqslant \log\delta^{-1} + \log\log\epsilon^{-1} + \log\beta + \frac{1}{2}. \tag{34}$$

To compute t_* and t^*, we may use Newton's method with initial values for the iteration satisfying (33)–(34). We also use the lemma to estimate the number of terms in S_F in Theorem 5. The proof of Lemma 7 is given in Appendix A.2.

The rate of decay of the integrand in (9)–(10) is much slower at $-\infty$ than at $+\infty$ and, for this reason, the equally spaced discretization S_F of the integral, although quite reasonable, still produces too many terms as the exponents e^{hn} in (21) become small (e.g., for negative n). As it was pointed out in [16], the number of terms in (21) may be reduced further. In Section 3 we provide a new simple method for this purpose.

2.2. Separated representation of e^{-xy} in terms of Gaussians

We may use Proposition 1 to obtain other useful approximations. As an example, let us consider the modified Bessel functions $\mathrm{K}_p(x)$ for positive argument x and complex order p. Using the integral representation [1, 9.6.24], we have

$$\mathrm{K}_p(xy) = \frac{1}{2}\int_0^\infty e^{-xy\cosh t}\left(e^{pt}+e^{-pt}\right)dt = \frac{1}{2}\int_{-\infty}^{\infty} e^{-xy\cosh t}e^{pt}\,dt = \frac{1}{2}\int_0^\infty e^{-xy(t+\frac{1}{t})/2}t^{p-1}\,dt, \tag{35}$$

for $x, y > 0$. Changing variables $t \mapsto x/yt$, we obtain

$$2^{p+1}\left(\frac{y}{x}\right)^p \mathrm{K}_p(xy) = \int_0^\infty e^{-x^2t/4-y^2t^{-1}}t^{p-1}\,dt = \int_{-\infty}^{\infty} e^{-x^2e^t/4-y^2e^{-t}+pt}\,dt. \tag{36}$$

Note that in this representation the variables x and y are separated and the integrand has a super-exponential decay at $\pm\infty$.

In particular, setting $p = 1/2$,

$$\mathrm{K}_{\frac{1}{2}}(x) = \left(\frac{\pi}{2}\right)^{\frac{1}{2}} x^{-\frac{1}{2}}e^{-x},$$

we obtain

$$e^{-xy} = \frac{x}{2\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-x^2e^t/4-y^2e^{-t}+\frac{1}{2}t}\,dt. \tag{37}$$

Defining

$$f(t) = \frac{x}{2\sqrt{\pi}}e^{-x^2e^t/4-y^2e^{-t}+\frac{1}{2}t}$$

and using (36), we have

$$\hat{f}(\xi) = \frac{x}{2\sqrt{\pi}}\int_{-\infty}^{\infty} e^{-x^2e^t/4-y^2e^{-t}+(\frac{1}{2}-2\pi\xi i)t}\,dt = \frac{x}{\sqrt{\pi}}\left(\frac{2y}{x}\right)^{\frac{1}{2}-2\pi\xi i}\mathrm{K}_{\frac{1}{2}-2\pi\xi i}(xy), \tag{38}$$

so that

$$\left|\hat{f}(\xi)\right| = \left(\frac{2}{\pi}\right)^{\frac{1}{2}}(xy)^{\frac{1}{2}}\left|\mathrm{K}_{\frac{1}{2}-2\pi\xi i}(xy)\right| = \left(\frac{2}{\pi}\right)^{\frac{1}{2}}(xy)^{\frac{1}{2}}\left|\mathrm{K}_{\frac{1}{2}+2\pi\xi i}(xy)\right|. \tag{39}$$

In order to use Proposition 1, we verify the exponential decay of $|\hat{f}(\xi)|$. Since $|\Gamma(1+yi)|^2 = \pi y/\sinh(\pi y)$ [1, 6.1.31], from [1, 9.6.25] we have

$$\left|\mathrm{K}_{\frac{1}{2}+2\pi\xi i}(x)\right| = \left(\frac{2}{\pi}\right)^{\frac{1}{2}}\left|\Gamma(1+2\pi\xi i)\right|x^{-\frac{1}{2}}\left|\int_0^\infty \frac{\cos(xt)}{(1+t^2)^{1+2\pi\xi i}}\,dt\right| \leqslant \left(\frac{\pi}{2}\right)^{\frac{1}{2}}x^{-\frac{1}{2}}\sqrt{\frac{2\pi^2\xi}{\sinh(2\pi^2\xi)}}.$$

Using Lemma 17 in Appendix A.4, we obtain for $x > 0$ and $\xi \in \mathbb{R}$,

$$\left|\mathrm{K}_{\frac{1}{2}+2\pi\xi i}(x)\right| \leqslant \left(\frac{\pi}{2}\right)^{\frac{1}{2}}3^{\frac{1}{4}}x^{-\frac{1}{2}}e^{-\frac{\pi^2}{2}|\xi|} \tag{40}$$

and, substituting in (39), arrive at

$$\left|\hat{f}(\xi)\right| \leqslant 3^{\frac{1}{4}}e^{-\frac{\pi^2}{2}|\xi|}.$$

Applying Proposition 1, an analysis similar to the one in Section 2.1 yields

Proposition 8. *For any $\delta > 0$, and $\epsilon > 0$, there exist a step size h and a positive integer M such that*

$$\left|e^{-xy} - G_e(x, y)\right| \leqslant \epsilon, \quad \text{for } xy \geqslant \delta, \tag{41}$$

where

$$G_e(x, y) = \frac{hx}{2\sqrt{\pi}} \sum_{j=0}^{M} e^{-\frac{x^2}{4}e^{s_j} - y^2 e^{-s_j} + \frac{1}{2}s_j} \tag{42}$$

and $s_j = s_{\text{start}} + jh$.

We note that (36) implies

$$\left|K_{\frac{1}{2}-2\pi\xi i}(x)\right| \leqslant K_{\frac{1}{2}}(x), \quad \text{for } x > 0,\ \xi \in \mathbb{R},$$

which, together with (40), yields a relative error estimate in (41).

Remark 9. In the two examples in Sections 2.1 and 2.2, we used particular integral representations to obtain approximations by exponentials. In both cases, the error estimates depend on considering the decay of certain functions on a vertical line in the complex plane. Namely, let us assume that the function $g(x)$ (which we are trying to approximate) is written as the Mellin transform, $\mathcal{M}$, of a function $u(x, \cdot)$,

$$g(x) = \int_0^\infty u(x, t)t^{p-1}\, dt = \big(\mathcal{M}u(x, \cdot)\big)(p),$$

where $p \in \mathbb{R}$ is some particular value which is the same for all x. By setting $t = e^s$, we also have

$$g(x) = \int_{-\infty}^{\infty} u\big(x, e^s\big)e^{ps}\, ds$$

and, following our approach, we compute the Fourier transform of the integrand,

$$\int_{-\infty}^{\infty} u\big(x, e^s\big)e^{ps-2\pi i\xi s}\, ds = \int_0^\infty u(x, t)t^{p-2\pi i\xi-1}\, dt = \big(\mathcal{M}u(x, \cdot)\big)(p - 2\pi i\xi).$$

This description holds in both (11) and (38) so that the approximation error in both cases depends on the behaviour of $(\mathcal{M}u(x, \cdot))(p - 2\pi i\xi)$ for large ξ.

3. A reduction scheme for sum of exponentials with small exponents

In Lemma 7, in truncating the infinite sum S_∞, we observe a substantially different behavior at the end points resulting in a relatively large number of terms with small exponents. As it was pointed out in [16], further reduction of the number of terms in S_F is possible. It turns out that for terms with small exponents a simple algorithm based on Prony's method is available and is described below.

Considering a sum of exponentials with small exponents,

$$f(x) = \sum_{m=1}^{M_0} \rho_m e^{\alpha_m x}, \tag{43}$$

where M_0 is large, our goal is to approximate $f(x)$ in $x \in [0, 1]$ by a shorter exponential sum with only $M \ll M_0$ terms. Since α_m are small, using the Taylor polynomial of degree $2M - 1$, we obtain

$$f(x) \approx \sum_{k=0}^{2M-1} h_k \frac{x^k}{k!} \tag{44}$$

with

$$h_k = \sum_{m=1}^{M_0} \rho_m \alpha_m^k, \quad k \geqslant 0. \tag{45}$$

We note that h_k is a fast decaying sequence so that $M \ll M_0$.

Below we show how to represent the first $2M$ terms of the sequence h_k as another exponential sum of only M terms,

$$h_k = \sum_{m=1}^{M} w_m \gamma_m^k, \quad 0 \leqslant k < 2M. \tag{46}$$

In this way, the coefficients h_k are now represented using $2M$ variables, the M coefficients w_m and the M distinct nodes γ_m, instead of the $2M_0$ variables in (45). Extending the representation (46) to all $k \geqslant 0$, we obtain our approximation to $f(x)$,

$$f(x) = \sum_{m=1}^{M_0} \rho_m e^{\alpha_m x} = \sum_{k=0}^{\infty} h_k \frac{x^k}{k!} \approx \sum_{k=0}^{\infty} \sum_{m=1}^{M} w_m \gamma_m^k \frac{x^k}{k!} = \sum_{m=1}^{M} w_m e^{\gamma_m x}.$$

To obtain the representation (46), we use Prony's method, which is related to our algorithm in Section 3 (see [16, Section 2.3]). Specifically, given $h_0, \ldots, h_{2M-1}$, we first find γ_m by obtaining the coefficients of the polynomial

$$q(z) = \prod_{m=1}^{M} (z - \gamma_m) = \sum_{k=0}^{M} q_k z^k.$$

Note that, for all k with $0 \leqslant k < M$,

$$\sum_{l=0}^{M} h_{k+l} q_l = \sum_{m=1}^{M} w_m \gamma_m^k \sum_{l=0}^{M} q_l \gamma_m^l = 0,$$

which also implies

$$\sum_{l=0}^{M-1} h_{k+l} q_l = -h_{M+k} \equiv b_k.$$

Thus, the vector $\mathbf{q} = (q_0, \ldots, q_{M-1})^t$ of the first M coefficients of $q(z)$, satisfies the linear system

$$\mathbf{Hq} = \mathbf{b} \tag{47}$$

where $\mathbf{H} = \{h_{k+l}\}_{k,l=0,\ldots,M-1}$ is an $M \times M$ Hankel matrix and $\mathbf{b} = (b_0, \ldots, b_{M-1})^t$.

The resulting algorithm consists of solving the system (47), forming the polynomial $q(z)$ and finding its roots γ_m. Using these roots we obtain the coefficients w_m by solving the Vandermonde system (46).

In Fig. 1 we illustrate the result of using this reduction algorithm by displaying the relative error of approximating the function $1/r^2$. In Table 1 we illustrate the relationship between accuracy and number of terms in the approximation of $r^{-\alpha}$, $\alpha = 1, 2, 3$ via Gaussians.

Remark 10. This reduction algorithm requires several properties to hold. The exponents α_k in (43) should be small enough as to warranty an effective reduction resulting in a small M. We also require the matrix $\mathbf{H}$ to be non-singular and the roots of $q(z)$ to be distinct. It is our observation that in all of our examples these properties are satisfied yielding a stable algorithm.

Remark 11. We note that the Taylor expansion may use an arbitrary center a,

$$e^{\alpha_m x} = \sum_{k=0}^{\infty} \frac{\alpha_m^k e^{\alpha_m a}}{k!} (x-a)^k$$

and, thus, the coefficients become

$$h_k = \sum_{m=1}^{M_0} \left(\rho_m e^{\alpha_m a}\right) \alpha_m^k = \sum_{m=1}^{M} \left(w_m e^{\gamma_m a}\right) \gamma_m^k.$$

4. Approximation of radial kernels by Gaussians

Many operators in mathematical physics depend only on the distance between interacting entities and, therefore, have radial kernels. By using Gaussians rather than exponentials (see Theorem 6) our approach leads to separated representations of positive radial kernels. We refer to [7,9,26,27,33,34], [13,14] and [11,12] for examples of using this approach on different operators.

Theorem 6 and Lemma 4 (applied to representations via Gaussians) provide useful tools for estimating the approximation error for kernels with singularities. As a representative example, let us consider the radial kernel $r^{-\alpha}$, $0 < \alpha < d$, where $r =$

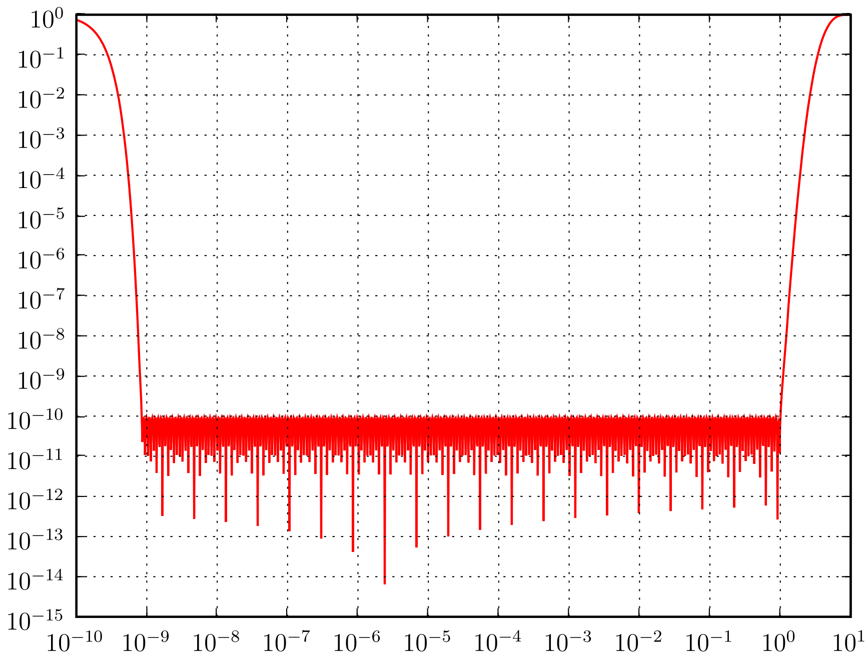

Fig. 1. Plot of the error $\log_{10}|1 - r^2 G_F(r)|$, where we have reduced the number of terms in G_F using the algorithm of Section 3. The reduced sum has 120 terms and achieves relative accuracy $\epsilon = 10^{-10}$ in the interval $[10^{-9}, 1]$.

Table 1
Relationship between accuracy ϵ and the number of terms in representations via Gaussians of $r^{-\alpha}$, $\alpha = 1, 2, 3$, for fixed $\delta = 10^{-9}$ after applying to G_F the reduction algorithm in Section 3. The dependence of the number of terms on accuracy appears to be almost linear in $\log \epsilon^{-1}$ rather than $\mathcal{O}((\log \epsilon^{-1})^2)$ as estimated in Theorem 6.

ϵ	$1/r$	$1/r^2$	$1/r^3$
10^{-6}	68	76	83
10^{-7}	79	88	93
10^{-8}	89	98	104
10^{-9}	100	109	116
10^{-10}	113	120	130

$\sqrt{\sum_{l=1}^{d} x_l^2}$. We are interested in applying the operator to compactly supported functions which, for simplicity, are rescaled to have support inside the box $D = [-1/2\sqrt{2}, 1/2\sqrt{2}]^d$. For $\mathbf{x} \in D$, we want to compute

$$(Tf)(\mathbf{x}) = \int_{\mathbb{R}^d} \|\mathbf{z} - \mathbf{x}\|^{-\alpha} f(\mathbf{z})\, d\mathbf{z} = \int_{\mathbb{R}^d} \|\mathbf{y}\|^{-\alpha} f(\mathbf{x} + \mathbf{y})\, d\mathbf{y} = \int_{B_1} \|\mathbf{y}\|^{-\alpha} f(\mathbf{x} + \mathbf{y})\, d\mathbf{y},$$

where B_r denotes the ball of radius r centered at $\mathbf{y} = \mathbf{0}$. We replace the kernel by its approximation via Gaussians constructed to be accurate in the interval $\delta \leqslant r \leqslant 1$ (see Theorem 6),

$$G_F(r) = G_F(r; M, N, h) = \frac{h}{\Gamma(\alpha/2)} \sum_{n=M+1}^{N} e^{h\alpha n/2} e^{-e^{hn} r^2}, \tag{48}$$

and estimate the resulting error. At issue is the impact of our approximation in the region $0 \leqslant r < \delta$, which in contrast with the kernel, has no singularity at $r = 0$. Next we derive an estimate which uses the fact that for all $r > 0$ the approximation is dominated by the true kernel (see Lemma 4).

Theorem 12. *Let* $0 < \alpha < d$ *and*

$$\left| r^{-\alpha} - G_F(r) \right| \leqslant \epsilon r^{-\alpha} \tag{49}$$

be an approximation of the kernel by Gaussians valid for $\delta \leqslant r \leqslant 1$. Then, for any bounded, compactly supported function f in D and $x \in D$, we have

$$\left| \int_{B_1} \|\mathbf{y}\|^{-\alpha} f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} - \int_{B_1} G_F\big(\|y\|\big) f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} \right| \leqslant \big(\epsilon + (2+\epsilon)\delta^{d-\alpha}\big)\frac{\omega_{d-1}}{d-\alpha}\|f\|_\infty.$$

Proof. Consider the ball B_δ of radius δ centered at $\mathbf{y}=\mathbf{0}$. Using (49), we have

$$\begin{aligned}\left| \int_{B_1\setminus B_\delta} \|\mathbf{y}\|^{-\alpha} f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} - \int_{B_1\setminus B_\delta} G_F\big(\|\mathbf{y}\|\big) f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} \right| &\leqslant \epsilon\left(\int_{B_1\setminus B_\delta} \|\mathbf{y}\|^{-\alpha}\, d\mathbf{y}\right)\|f\|_\infty \\ &\leqslant \epsilon\left(\int_{B_1} \|\mathbf{y}\|^{-\alpha}\, d\mathbf{y}\right)\|f\|_\infty = \epsilon\frac{\omega_{d-1}}{d-\alpha}\|f\|_\infty,\end{aligned}$$

where $\omega_{d-1} = 2\pi^{d/2}/\Gamma(d/2)$ is the surface area of the unit sphere in $\mathbb{R}^d$. Using Lemma 4, we obtain

$$\begin{aligned}\left| \int_{B_\delta} \|\mathbf{y}\|^{-\alpha} f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} - \int_{B_\delta} G_F\big(\|\mathbf{y}\|\big) f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} \right| &\leqslant \int_{B_\delta} \big| \|\mathbf{y}\|^{-\alpha} - G_F\big(\|\mathbf{y}\|\big)\big|\, d\mathbf{y}\, \|f\|_\infty \\ &\leqslant (2+\epsilon)\int_{B_\delta} \|\mathbf{y}\|^{-\alpha} d\mathbf{y}\, \|f\|_\infty = (2+\epsilon)\frac{\omega_{d-1}\delta^{d-\alpha}}{d-\alpha}\|f\|_\infty. \qquad \square\end{aligned}$$

Using Lemma 4 as in Theorem 12 simplifies and corrects proofs given in [9]. In [9] it is sufficient to use Eq. (24), Eq. (57) and Lemma 4, while Eq. (25) and Eq. (58) are in error and should be ignored.

Since the number of terms depends logarithmically on δ, Theorem 12 provides a good control of error. Further improvement may be achieved by observing that, as we approach the singularity at $r=0$, N becomes large in (48) so that we add more terms with large exponents. Assuming that f is sufficiently smooth, as exponents become large, the contribution of corresponding terms may be evaluated explicitly removing the dependence on δ in Theorem 12. We have

Theorem 13. *Let $0 < \alpha < d$ and consider the approximation valid for $0 < r \leqslant 1$,*

$$\big| r^{-\alpha} - G_F(r; M, \infty, h)\big| \leqslant \epsilon r^{-\alpha}, \tag{50}$$

where G_F is given in (48). Then, for a bounded, sufficiently smooth, compactly supported function f in D, we have for all $\mathbf{x} \in D$

$$\left| \int_D \|\mathbf{x}-\mathbf{y}\|^{-\alpha} f(\mathbf{y})\, d\mathbf{y} - \int_D G_F\big(\|\mathbf{x}-\mathbf{y}\|; M, \infty, h\big) f(\mathbf{y})\, d\mathbf{y} \right| \leqslant \epsilon\frac{\omega_{d-1}}{d-\alpha}\|f\|_\infty$$

and, for sufficiently large N,

$$\begin{aligned}\int_D G_F\big(\|\mathbf{x}-\mathbf{y}\|; M, \infty, h\big) f(\mathbf{y})\, d\mathbf{y} &= \int_D G_F\big(\|\mathbf{x}-\mathbf{y}\|; M, N-1, h\big) f(\mathbf{y})\, d\mathbf{y} \\ &\quad + C_0 f(\mathbf{x}) e^{h(\alpha-d)N/2} + C_2 \Delta f(\mathbf{x}) e^{h(\alpha-d-2)N/2} + \mathcal{O}\big(e^{h(\alpha-d-4)N/2}\big),\end{aligned} \tag{51}$$

where Δ is the Laplacian and

$$C_0 = \frac{h\pi^{d/2}}{\Gamma(\alpha/2)(1-e^{h(\alpha-d)/2})} \quad \textit{and} \quad C_2 = \frac{h\pi^{d/2}}{4\Gamma(\alpha/2)(1-e^{h(\alpha-d-2)/2})}.$$

Proof. From (26) in Theorem 6, we obtain

$$\begin{aligned}\left| \int_{B_1} \|\mathbf{y}\|^{-\alpha} f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} - \int_{B_1} G_\infty\big(\|\mathbf{y}\|\big) f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} \right| &\leqslant \epsilon\left(\int_{B_1} \|\mathbf{y}\|^{-\alpha}\, d\mathbf{y}\right)\|f\|_\infty \\ &= \epsilon\frac{\omega_{d-1}}{d-\alpha}\|f\|_\infty,\end{aligned}$$

where

$$G_\infty(r) = G_F(r; M, \infty, h) = \frac{h}{\Gamma(\alpha/2)} \sum_{n=M+1}^{\infty} e^{\alpha hn/2} e^{-e^{hn} r^2}. \tag{52}$$

Extending integration to the whole space and splitting the series (52) for a sufficiently large N, we have

$$\int_{B_1} G_\infty\big(\|\mathbf{y}\|\big) f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} = \int_{\mathbb{R}^d} G_F\big(\|\mathbf{y}\|; M, N-1, h\big) f(\mathbf{x}+\mathbf{y})\, d\mathbf{y} + \frac{h}{\Gamma(\alpha/2)} \sum_{n=N}^{\infty} e^{h\alpha n/2} \int_{\mathbb{R}^d} e^{-e^{hn}\|\mathbf{y}\|^2} f(\mathbf{x}+\mathbf{y})\, d\mathbf{y}. \tag{53}$$

Using the Taylor expansion

$$f(\mathbf{x}+\mathbf{y}) = f(\mathbf{x}) + \nabla f(\mathbf{x}) \cdot \mathbf{y} + \frac{1}{2}\big\langle H(\mathbf{x})\mathbf{y}, \mathbf{y}\big\rangle + \mathcal{O}\big(\|\mathbf{y}\|^3\big), \tag{54}$$

where $H(\mathbf{x})$ is the Hessian matrix $\{f_{y_i y_j}(\mathbf{x})\}_{i,j=1,\dots,d}$, we evaluate the contribution of each term in (53). For the first term in (54), we have

$$f(\mathbf{x}) \sum_{n=N}^{\infty} \frac{h}{\Gamma(\alpha/2)} e^{h\alpha n/2} \int_{\mathbb{R}^d} e^{-e^{hn}\|\mathbf{y}\|^2}\, d\mathbf{y} = f(\mathbf{x}) \frac{h\pi^{d/2}}{\Gamma(\alpha/2)} \sum_{n=N}^{\infty} e^{h(\alpha-d)n/2} = C_0 f(\mathbf{x}) e^{h(\alpha-d)N/2}.$$

Observing that the second term and the non-diagonal entries of the third term in (54) do not contribute due to parity, we have

$$\begin{aligned}\sum_{n=N}^{\infty} \frac{h}{2\Gamma(\alpha/2)} \sum_{i=1}^{d} f_{y_i y_i}(\mathbf{x}) e^{h\alpha n/2} \int_{\mathbb{R}^d} e^{-e^{hn}\|\mathbf{y}\|^2} y_i^2\, d\mathbf{y} &= \Delta f(\mathbf{x}) \frac{h\pi^{d/2}}{4\Gamma(\alpha/2)} \sum_{n=N}^{\infty} e^{h(\alpha-d-2)n/2} \\ &= C_2 \Delta f(\mathbf{x}) e^{h(\alpha-d-2)N/2},\end{aligned}$$

which has the extra factor e^{-hN} in comparison with the first term. We may continue this process using more terms in (54) to obtain the asymptotic expansion in (51). □

5. Multiresolution representation of solutions of Laplace's equation and its application to gravity modeling

5.1. Spherical harmonic gravity models

Current models of gravitational potentials use solutions of Laplace's equation in the exterior of a sphere as a template for model representation. For example, the spherical harmonic model of order and degree N of the Earth's gravitational potential is of the form

$$U(\rho, \phi, \theta) = \frac{\mu}{R\rho}\left(1 + \sum_{n=1}^{N} \rho^{-n} \sum_{m=0}^{n} \bar{P}_n^m(\cos\theta)\big(\bar{c}_n^m \cos(m\phi) + \bar{s}_n^m \sin(m\phi)\big)\right), \tag{55}$$

where μ is the gravitational constant, R is the equatorial radius of the Earth, ϕ is the geocentric longitude and θ is the geocentric latitude. In (55) the functions $\bar{P}_n^m$ are normalized associated Legendre functions of degree n and order m, $\bar{c}_n^m$, $\bar{s}_n^m$, $n = 1, \dots, N$, are normalized coefficients of the model and $\rho = r/R \geqslant 1$ is the dimensionless distance. Such models are used to evaluate forces for computation of satellite orbits (see [24]). A similar representation is used in constructing gravitational potentials for other celestial bodies, e.g. the Moon.

One of the difficulties in using the spherical harmonic models for evaluating forces is the $\mathcal{O}(N^2)$ cost of their evaluation at a single point (ρ, ϕ, θ). This cost may be significantly reduced by creating local approximations to U on a collection of spheres of different radii and interpolating between them (see [8]). Another set of issues arises in the construction of such gravity models due to the global nature of the representation (55). In particular, since gravity measurements collected at different distances from the surface of the Earth account for a different spatial resolution, it is difficult to use such measurements in a simultaneous estimation of the coefficients in (55).

Using the approximation via Gaussians of Sections 2.1 and 2.2, we introduce a multiresolution reorganization of (55). This new representation in combination with local approximation on spheres in [8] or in [2] provides a theoretical foundation for a new approach to evaluate and estimate the gravitational potential or other fields associated with massive or charged bodies.

5.2. Laplace's equation in a half-space

In order to illustrate the use of Gaussians in obtaining a multiresolution approximation of solutions of boundary value problems for Laplace's equation, we first describe such construction for the half-space. In the next section we develop a similar approximation for the problem with boundary conditions on a sphere.

A harmonic function $u(z,\mathbf{x})$ in the upper half-space $z>0$, satisfying $u_{zz}+\Delta_{\mathbf{x}}u=0$ and $u(0,\mathbf{x})=u_0(\mathbf{x})$, may be written as

$$u(z,\mathbf{x})=\int_{\mathbb{R}^d}\mathcal{P}(z,\mathbf{x}-\mathbf{y})u_0(\mathbf{y})\,d\mathbf{y},\quad z\geqslant 0,\tag{56}$$

where

$$\mathcal{P}(z,\mathbf{x})=\frac{2}{\omega_d}\frac{z}{(z^2+\|\mathbf{x}\|^2)^{(d+1)/2}}$$

is the Poisson kernel for the upper half-space. Using Theorem 3, for any $\epsilon>0$ and $z>0$, we approximate the Poisson kernel with

$$S_\infty\big(z^2+\|\mathbf{x}\|^2\big)=\frac{zh}{\pi^{(d+1)/2}}\sum_{j\in\mathbb{Z}}e^{(d+1)hj/2}e^{-e^{hj}z^2}e^{-e^{hj}\|\mathbf{x}\|^2}.\tag{57}$$

Substituting (57) in (56), we obtain an approximation

$$\tilde{u}(z,\mathbf{x})=\frac{zh}{\pi^{(d+1)/2}}\sum_{j\in\mathbb{Z}}e^{(d+1)hj/2}e^{-e^{hj}z^2}W_j(\mathbf{x}),\tag{58}$$

where

$$W_j(\mathbf{x})=\int_{\mathbb{R}^d}e^{-e^{hj}\|\mathbf{x}-\mathbf{y}\|^2}u_0(\mathbf{y})\,d\mathbf{y}.\tag{59}$$

The structure of the separated representation (58)–(59) is such that, for large z, the contribution to (58) is significant only for small e^{hj}. For such exponents, due to the convolution with the corresponding Gaussian, W_j contains only low spatial frequencies. As z becomes small, higher and higher spatial frequencies contribute to $\tilde{u}$. Hence, the separated representation (58)–(59) has a multiresolution structure that may be exploited in obtaining fast algorithms (see e.g. [7]).

5.3. Laplace's equation with boundary values on a sphere

A harmonic function $U(r/R,\phi,\theta)$ outside a sphere of radius R with the boundary condition $U(1,\phi,\theta)=v(\phi,\theta)$ may be represented as

$$U(\rho,\phi,\theta)=\sum_{n=0}^{\infty}\rho^{-n-1}U_n(\phi,\theta),\tag{60}$$

where $\rho=r/R\geqslant 1$ and

$$U_n(\phi,\theta)=\frac{2n+1}{4\pi}\int_0^{2\pi}\int_0^{\pi}P_n(\cos\gamma)v(\phi',\theta')\sin\theta'\,d\theta'\,d\phi'.$$

Here P_n are the Legendre polynomials and

$$\cos\gamma=\cos\theta\cos\theta'+\sin\theta\sin\theta'\cos(\phi-\phi').$$

Setting $x=n$, $n\geqslant 1$, and $y=\log\rho$, $\rho>1$, in (37), we obtain

$$\rho^{-n}=e^{-n\log\rho}=\frac{n}{2\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-n^2e^{-t}/4-(\log\rho)^2e^t-t/2}\,dt.\tag{61}$$

Discretizing (61) with a sufficiently small step size h, we obtain

$$\big|\rho^{-n}-G_{e,\infty}(n,\log\rho,h)\big|\leqslant\epsilon,\tag{62}$$

where

$$\begin{aligned}G_{e,\infty}(n,\log\rho,h)&=\frac{hn}{2\sqrt{\pi}}\sum_{j\in\mathbb{Z}}e^{-n^2e^{-jh}/4-(\log\rho)^2e^{jh}-jh/2}\\&=\frac{hn}{\sqrt{2\pi}}\sum_{j\in\mathbb{Z}}\sigma_j^{-1}e^{-n^2/(2\sigma_j^2)}e^{-(\log\rho)^2\sigma_j^2/2}\end{aligned}\tag{63}$$

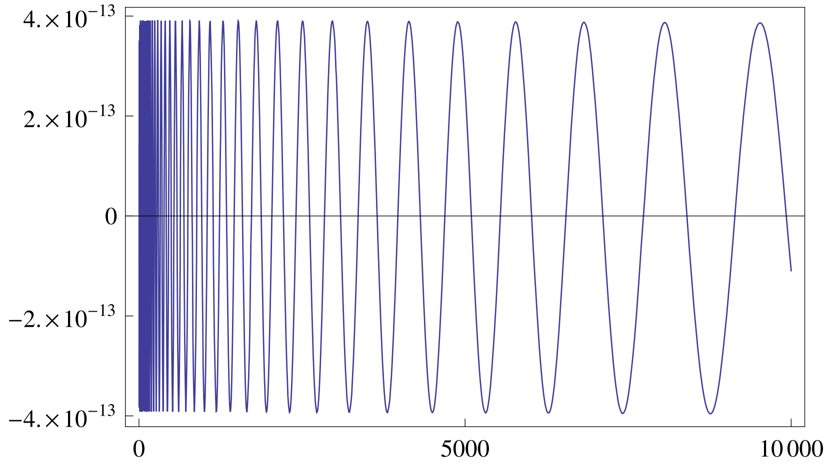

Fig. 2. Error for $2 \leqslant n \leqslant 10{,}000$ in (62), where the infinite sum $G_{e,\infty}$ has been truncated and has only terms with $j = -10, \ldots, 70$ and $h = 1/3$. The error is computed for a fixed $\rho = 1 + \delta$, with $\delta = 1/(4 \cdot 6378)$ (corresponding to a position approximately 250 meters above the Earth's surface using as its equatorial radius $R \approx 6378$ km). We note that for larger δ we need to keep even fewer terms in (63) yielding a better absolute error than the one illustrated here.

with $\sigma_j^2 = 2e^{jh}$. Substituting these approximations into (60), we obtain an approximation to U of the form

$$\tilde{U}(\rho, \phi, \theta) = \sum_{j \in \mathbb{Z}} e^{-(\log \rho)^2 \sigma_j^2/2} Z_j(\phi, \theta), \tag{64}$$

where

$$Z_j(\phi, \theta) = \frac{h}{\sigma_j \sqrt{2\pi}} \sum_{n=0}^{\infty} (n+1) e^{-(n+1)^2/(2\sigma_j^2)} U_n(\phi, \theta). \tag{65}$$

The separated representation (64)–(65) has a multiresolution structure similar to that of the solution of the Laplace's equation in the half-space. For a fixed accuracy $\epsilon > 0$ and a fixed σ_j, we need to retain only a finite number of terms in (65) due to the factor $e^{-(n+1)^2/(2\sigma_j^2)}$ in the definition of $Z_j(\phi, \theta)$. At the same time, depending on the size of $\log \rho$, only a limited number of terms in (64) are significant. In other words, functions $Z_j(\phi, \theta)$ with high spatial resolution are needed only for ρ close to 1, and for large ρ we need only $Z_j(\phi, \theta)$ with a low spatial resolution. We note that by limiting the range of ρ, the series in (64) may be replaced by a finite sum where the number of terms may be reduced using the algorithm in Section 3. The approximation error in (62) is illustrated in Fig. 2.

Besides fast evaluation of forces for orbit computations, we intend to use (64)–(65) for constructing gravity models. Note that we may estimate the functions $Z_j(\phi, \theta)$ in (65) from measurements (of the gravitational potential or quantities associated with it) as opposed to estimating the coefficients in (55). The advantage of this approach is that, for a given accuracy ϵ, we know in advance the required resolution to represent $Z_j(\phi, \theta)$ for a particular parameter σ_j. Specifically, measurements taken at different distances from the Earth's surface and having different spatial resolutions, are involved in the estimation of only specific terms $Z_j(\phi, \theta)$. Thus, the estimation of $Z_j(\phi, \theta)$ for different j may be done hierarchically, in a semi-independent manner. This should be compared with the standard representation via spherical harmonics (55), where a typical estimation solves for all coefficients in (55) simultaneously. We note that our goal in this paper is limited to demonstrating feasibility of using separated representations in (64)–(65) for gravity modeling, while it is clear that much more work is required to demonstrate further practical advantages of the approach in order for it to compete with existing methods of gravity estimation.

Appendix A

A.1. Algorithm for approximations by sum of exponentials

We briefly review the algorithm in [16] to approximate functions by sum of exponentials. These approximations, obtained for a finite but arbitrary accuracy, have significantly fewer terms than corresponding Fourier representations (see [15–17]).

Given $\epsilon > 0$ and $2N + 1$ values of the complex-valued function $h(a\xi)$ on a uniform grid in $[0, 1]$, we have developed in [16] an algorithm to obtain complex coefficients w_m and exponents t_m, and (nearly) minimal $M = M(\epsilon, a)$ such that

$$\left| h\left(a \frac{n}{2N}\right) - \sum_{m=1}^{M} w_m e^{-t_m n} \right| < \epsilon, \tag{66}$$

for any $0 \leqslant n \leqslant 2N$. In this formulation, $a > 0$ scales the problem to the interval $[0, 1]$ and ϵ is the accuracy sought.

Using coefficients w_m in (66) and exponents $\eta_m = \frac{2N}{a} t_m$, we have an approximation to $h(x)$ by a sum of exponentials valid for all $x \in [0, a]$,

$$\left| h(x) - \sum_{m=1}^{M} w_m e^{-\eta_m x} \right| < \epsilon', \tag{67}$$

where ϵ' is very close to ϵ provided that the function h is appropriately sampled in (66) to justify local interpolation.

The steps to achieve the approximation (66) are as follows:

- Build the $(N+1) \times (N+1)$ Hankel matrix $\mathbf{H}_{kl} = h_{k+l}$ using the samples $h_n = h(a\frac{n}{2N})$, $0 \leqslant n \leqslant 2N$.
- Find a vector $\mathbf{u} = (u_0, \ldots, u_N)$, satisfying $\mathbf{Hu} = \sigma \bar{\mathbf{u}}$, with positive σ close to the target accuracy ϵ. The existence of such vector $\mathbf{u}$ follows from Tagaki's factorization (see [16, p. 22]); the singular value decomposition yields σ as a singular value and $\mathbf{u}$ as a singular vector of $\mathbf{H}$. We label the first $M+1$ singular values of $\mathbf{H}$ in decreasing order $\sigma_0 \geqslant \sigma_1 \geqslant \cdots \geqslant \sigma_M$, where σ_M is chosen so that $\sigma_M/\sigma_0 \approx \epsilon$. Typically, singular values decay rapidly and, thus, $M = \mathcal{O}(\log \epsilon^{-1})$ and $M \ll N$.
- Compute roots γ_m of the polynomial $u(z) = \sum_{n=0}^{N} u_n z^n$ whose coefficients are the entries of the singular vector $\mathbf{u}$ computed in the previous step. The coefficients w_m are obtained solving the least-squares Vandermonde system

  $$\sum_{m=1}^{N} w_m \gamma_m^n = h\left(a \frac{n}{2N}\right), \quad 0 \leqslant n \leqslant 2N.$$

  Typically, only M coefficients w_m have absolute value larger than the target accuracy ϵ, thus allowing us to remove most roots γ_m from further consideration. It is often possible to predict the approximate location of roots γ_m with significant coefficients and, thus, find only them. However, if no a priori information on their location is available, then all roots should be computed and selected according to the size of the corresponding coefficients. In those rare cases where the polynomial $u(z)$ has multiple roots, a small perturbation of the matrix $\mathbf{H}$ provides a way to obtain a perturbed polynomial with simple roots, a property required by the representation we seek.
- The exponents t_m in (66) correspond to $t_m = \log \gamma_m$, where log is the principal value of the logarithm.

For more details on this algorithm we refer to [16]. We note that the special case of purely imaginary exponents η_m in (67) is treated in [15]. For properties of approximations by exponential sums with real exponents see [19, Chapter 6].

A.2. Proof of Lemma 7

Let

$$g(t) = 1 - \frac{\Gamma(\beta, e^t)}{\Gamma(\beta)} = \frac{1}{\Gamma(\beta)} \int_{-\infty}^{t} e^{-e^y + \beta y} \, dy.$$

We have

$$g(t) \leqslant \frac{1}{\Gamma(\beta)} \int_{-\infty}^{t} e^{\beta y} \, dy = \frac{e^{\beta t}}{\Gamma(1+\beta)},$$

and defining our estimate $\tilde{t}_*$ for the lower value t_* as

$$\tilde{t}_* = \frac{\log \epsilon \Gamma(1+\beta)}{\beta} = \frac{1}{\beta} \log \epsilon + \log \Gamma(1+\beta)^{\frac{1}{\beta}}, \tag{68}$$

we have $g(\tilde{t}_*) \leqslant \epsilon = g(t_*)$. Since g is an increasing function, it follows that $\tilde{t}_* \leqslant t_*$.

To estimate t^* in (32), note that if we bound $u(t) = \Gamma(\beta, \delta e^t)/\Gamma(\beta) \leqslant U(t)$ and define $\tilde{t}^*$ such that $U(\tilde{t}^*) = \epsilon$, we have $u(\tilde{t}^*) \leqslant U(\tilde{t}^*) = u(t^\star)$. Since u is a decreasing function, it follows that $t^\star \leqslant \tilde{t}^*$. To bound $u(t)$, we use that (see [31, Section 3.1])

$$\Gamma(\beta, x) \leqslant \begin{cases} x^{\beta-1} e^{-x}, & \text{for } 0 < \beta \leqslant 1, \ x > 0, \\ e x^{\beta-1} e^{-x}, & \text{for } \beta > 1, \ x > \frac{e}{e-1}(\beta - 1). \end{cases} \tag{69}$$

Let $x = \delta e^t$ and assume $x \geqslant 1$, i.e., $t \geqslant \log \delta^{-1}$. We first consider the case $0 < \beta \leqslant 1$, which implies $x^{\beta-1} \leqslant 1$ and $1 \leqslant \Gamma(\beta)$ and thus

$$\frac{\Gamma(\beta, x)}{\Gamma(\beta)} \leqslant \frac{1}{\Gamma(\beta)} x^{\beta-1} e^{-x} \leqslant e^{-x} = \epsilon$$

if we choose $x = \log \epsilon^{-1}$. Thus, our estimate for this range of β is

$$\tilde{t}^* = \log \delta^{-1} + \log \log \epsilon^{-1}. \tag{70}$$

If $\beta > 1$, we have

$$\frac{\Gamma(\beta, x)}{\Gamma(\beta)} \leqslant \frac{e}{\Gamma(\beta)} x^{\beta-1} e^{-x} \leqslant \epsilon,$$

where the first inequality holds using (69) with

$$x > d(\beta - 1) \tag{71}$$

where $d = e/(e-1) \approx 1.582$, and the second holds if, using Lemma 14, we consider a positive x such that

$$x \geqslant d\left[(\beta - 1)\log(\beta - 1) - \log \Gamma(\beta) + \log e\epsilon^{-1}\right]. \tag{72}$$

To simplify the last inequality, we use the results in [3] which imply that, for $1 < \beta \leqslant 2$,

$$(\beta - 1)\log(\beta - 1) - \log \Gamma(\beta) \leqslant 0.$$

Since $\epsilon \leqslant 1$, we select $x = d \log(e\epsilon^{-1}) > d(\beta - 1)$ which satisfies both (71) and (72). Therefore, our estimate becomes

$$\tilde{t}^* = \log d\delta^{-1} + \log \log e\epsilon^{-1}. \tag{73}$$

For $\beta > 2$, we use

$$y^{y+1-\gamma} e^{1-y} < \Gamma(y + 1) \tag{74}$$

where $y > 1$ and $\gamma = 0.577\ldots$ is the Euler's constant [29]. Substituting $y = \beta - 1$ in (74) yields

$$(\beta - 1)\log(\beta - 1) - \log \Gamma(\beta) < (\gamma - 1)\log(\beta - 1) + \beta - 2 < \beta - 2.$$

By selecting $x = d(\beta - 1 + \log \epsilon^{-1}) > d(\beta - 1)$ we satisfy (71) and (72). Hence, for $\beta > 2$

$$\tilde{t}^* = \log d\delta^{-1} + \log\left(\beta - 1 + \log \epsilon^{-1}\right). \tag{75}$$

To simplify $\tilde{t}^*$, we collect our previous estimates (70), (73), and (75) in a single estimate now valid for all $\beta > 0$,

$$\log\left(\delta^{-1}\right) + \log\left(\log \epsilon^{-1} + \beta\right) + \frac{1}{2} \leqslant \log \delta^{-1} + \log \log \epsilon^{-1} + \log \beta + \frac{1}{2},$$

where, for the last inequality, we used $\epsilon \leqslant 1/e$.

Next lemma is a refinement of Lemma A.3 in [16].

Lemma 14. *Let p, x and ϵ be positive numbers and define $c = \log p\epsilon^{-1/p}$. If $x > 0$ and $c \leqslant 1$ or, alternatively, $x \geqslant (p \log p + \log \epsilon^{-1})e/(e-1) = pce/(e-1)$ and $c > 1$, then the inequality*

$$x^p e^{-x} \leqslant \epsilon \tag{76}$$

holds.

Proof. Inequality (76) is equivalent to

$$\log \epsilon^{-\frac{1}{p}} \leqslant \frac{x}{p} - \log x,$$

or, with $y = \frac{x}{p}$,

$$c \leqslant y - \log y = g(y). \tag{77}$$

Since $g(y) \geqslant 1$ for all positive y and it is an increasing function for $y \geqslant 1$, under the condition $x > 0$ and $c \leqslant 1$ the result follows. For the second condition, we write $y = dc$, with $d = e/(e-1) > 1$. Then, we have $y > 1$ which satisfies (77) since, for all positive t,

$$\log t \leqslant \frac{1}{e} t = \left(1 - \frac{1}{d}\right) t,$$

and, thus,

$$c + \log y \leqslant c + \frac{y}{e} = dc = y. \qquad \square$$

A.3. Proof of Theorem 5

In Section 2.1.1 we have already shown how to obtain (20) for some h satisfying (15) and t_* and t^* satisfying Lemma 7. To simplify the approximation, we set $t_0 = 0$ and

$$\tilde{h} = \frac{10}{2\log\epsilon^{-1} + \log\beta + 2}.$$

To estimate the number of terms, it is enough to bound

$$\frac{\tilde{t}^* - \tilde{t}_*}{\tilde{h}},$$

where $\tilde{t}^*$, $\tilde{t}_*$ are the bounds in (33) and (34). We have

$$\begin{aligned}\tilde{t}^* - \tilde{t}_* &= \log\delta^{-1} + \frac{1}{\beta}\log\epsilon^{-1} + \log\log\epsilon^{-1} + \log\left(\frac{\beta+1}{\Gamma(1+\beta)^{\frac{1}{\beta}}}\right) + \frac{1}{2}\\ &\leqslant \log\delta^{-1} + \frac{1}{\beta}\log\epsilon^{-1} + \log\log\epsilon^{-1} + \frac{3}{2}\end{aligned}$$

where we used Lemma 15.

The estimate (23) follows from (27)–(28).

Lemma 15. *Let $g(x) = \frac{\Gamma(x+1)^{\frac{1}{x}}}{x+1}$ for $x > 0$. The function g is always decreasing and for all $x > 0$,*

$$e^{-1} \leqslant g(x) \leqslant e^{-\gamma}, \tag{78}$$

where $\gamma = 0.577\ldots$ is the Euler's constant. In particular,

$$\log\frac{x+1}{\Gamma(x+1)^{\frac{1}{x}}} \leqslant 1 \quad \text{for } x > 0. \tag{79}$$

Proof. Considering the logarithmic derivative of g and denoting $\psi(x) = \Gamma'(x)/\Gamma(x)$, is enough to show that

$$p(x) = x^2(\log g)'(x) = x\psi(x+1) - \log\Gamma(x+1) - \frac{x^2}{x+1}$$

is always negative. Since $p(0) = 0$, we simply show that $p'(x) = x\psi'(x+1) - 1 + (x+1)^{-2} \leqslant 0$, or equivalently, that

$$\psi'(y) \leqslant y^{-1} + y^{-2}, \tag{80}$$

for $y \geqslant 1$. In fact, (80) is valid for any $y > 0$ as may be seen using the representation [1, 6.4.10]

$$\psi'(y) = \sum_{k=0}^{\infty}\frac{1}{(y+k)^2}, \quad y > 0,$$

which implies

$$\psi'(y) - y^{-2} \leqslant \int_0^{\infty}\frac{1}{(y+t)^2}\,dt = \frac{1}{y},$$

where we used that $t \mapsto (y+t)^{-2}$ is positive and decreasing. To obtain (78), we note that

$$\lim_{x\to 0^+} g(x) = e^{\lim_{x\to 0}\frac{\log\Gamma(x+1)}{x} - \log(x+1)} = e^{\psi(1)} = e^{-\gamma}$$

while $\lim_{x\to\infty} g(x) = e^{-1}$ follows from [1, 6.1.38]. □

Remark 16. In [22, Theorem 1.1] it is shown that the function $g(x)$ in Lemma 15 is decreasing for $x \geqslant 1$ while the results in [4, Theorem 3.2] imply that a related function, $\Gamma(1+x)^{1/x}/x$ is decreasing for $x > 0$.

A.4. An estimate for the derivation of (40)

Lemma 17. *For all $y \in \mathbb{R}$,*

$$\frac{y}{\sinh y} \leqslant \sqrt{3} e^{-\frac{1}{2}|y|}. \tag{81}$$

Proof. It is sufficient to show (81) for $y > 0$, or equivalently, with the substitution $x = e^{y/2}$, show that

$$\frac{4}{\sqrt{3}} \log x \leqslant x - x^{-3} = x^{-1}\left(x^2 - x^{-2}\right) \quad \text{for } x \geqslant 1.$$

Let

$$g(x) = x - x^{-3} - \frac{4}{\sqrt{3}} \log x$$

and note that

$$g'(x) = 3x^{-4} - \frac{4}{\sqrt{3}} x^{-1} + 1 = 3\left(x^{-1} - \frac{1}{\sqrt{3}}\right)^2 \left(x^{-2} + \frac{2}{\sqrt{3}} x^{-1} + 1\right) \geqslant 0$$

and $g(1) = 0$. □

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