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Appl. Comput. Harmon. Anal. 19 (2005) 17–48

**Applied and
Computational
Harmonic Analysis**

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On approximation of functions by exponential sums[☆]

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Received 21 September 2004; accepted 24 January 2005

Available online 31 March 2005

Communicated by Charles K. Chui

Abstract

We introduce a new approach, and associated algorithms, for the efficient approximation of functions and sequences by short linear combinations of exponential functions with complex-valued exponents and coefficients. These approximations are obtained for a finite but arbitrary accuracy and typically have significantly fewer terms than Fourier representations. We present several examples of these approximations and discuss applications to fast algorithms. In particular, we show how to obtain a short separated representation (sum of products of one-dimensional functions) of certain multi-dimensional Green's functions.

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Keywords: Exponential sums; Hankel matrices; Prony's method; Separated representations

1. Introduction

We consider the problem of approximating functions on a finite real interval by linear combination of exponentials with complex-valued exponents and discuss several applications of these approximations. The approximations we obtain in this paper are already being used for constructing Green's functions in quantum chemistry and fluid dynamics [8,15,16], and we expect further applications in computing lattice sums, approximating Green's functions in electromagnetics, and addressing some problems of signal

[☆] This research is partially supported by NSF/ITR Grant DMS-0219326, DOE Grant DE-FG02-03ER25583, and DARPA/ARO Grant W911NF-04-1-0281.

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processing and data compression. In this paper we prove new theoretical results and develop numerical algorithms for constructing such approximations. Since our numerical results are far better than our current proofs indicate, we also point out unresolved issues in this emerging theory.

Since our formulation is somewhat unusual, we first provide two examples. Let us consider the identity

$$\frac{1}{x} = \int_0^{\infty} e^{-tx} dt \quad (1)$$

for $x > 0$. This integral representation readily leads to an approximation of the function $\frac{1}{x}$ as a sum of exponentials. In fact, for any fixed $\varepsilon > 0$, there exist positive weights and nodes (exponents) of the generalized Gaussian quadrature such that

$$\left| \frac{1}{x} - \sum_{m=1}^M w_m e^{-t_m x} \right| \leq \frac{\varepsilon}{x} \quad (2)$$

for all x in a finite interval, $0 < \delta \leq x \leq 1$, and where the number of terms is $M = \mathcal{O}(\log \delta)$. Theoretically the existence of such approximations follows from [19–22]. This particular example has been examined in [27] with the goal of using (2) for constructing fast algorithms. Specific exponents and weights are provided there for several intervals and values of ε , so that (2) can be verified explicitly. The approximation (2) has important applications to fast algorithms that we will consider below.

The second example is the Bessel function $J_0(bx)$, where $b > 0$ is a parameter and $x \in [0, 1]$. Using the approach developed in this paper, we obtain for all x on $[0, 1]$,

$$\left| J_0(bx) - \sum_{m=1}^M \rho_m e^{\tau_m x} \right| \leq \varepsilon, \quad (3)$$

where ρ_m and τ_m are now complex numbers and the number of terms, M , is remarkably small and increases with b and ε as $M = \mathcal{O}(\log b) + \mathcal{O}(\log \varepsilon^{-1})$. In the sum (3) we will refer to the coefficients ρ_m as weights and to the values e^{τ_m} as nodes; such terminology is natural since, as it turns out, e^{τ_m} are zeros of a certain polynomial as is usually the case for quadratures. We illustrate (3) in Figs. 1 and 2 by showing the error of the approximation and the location of the weights ρ_m and (normalized) nodes $e^{\tau_m/b}$ corresponding to $b = 100\pi$ and $\varepsilon \simeq 10^{-11}$. The number of nodes is $M = 28$ and they accumulate at e^i and e^{-i} as expected from the form of the approximation in (3) and the asymptotics of J_0 for large argument,

$$J_0(b) \sim \frac{(1-i)e^{ib} + (1+i)e^{-ib}}{2\sqrt{\pi b}}.$$

Also, since the real part of the exponents is always negative, $\text{Re}(\tau_m) < 0$, all nodes belong to the unit disk. The approximation (3) with these 28 terms is remarkable in that there is no obvious integral, as in (1), to represent the function and, thus, by some quadrature, obtain so few terms for a given accuracy and parameter b . Clearly, there are many possible integrals in the complex plane to represent the Bessel function but, unfortunately, there is no obvious criteria to choose a particular integral or contour. Finding such a contour may be attempted via the steepest descent method, in this case starting from, e.g.,

$$J_0(bx) = \frac{1}{\pi} \int_{-1}^1 \frac{e^{ibxt}}{\sqrt{1-t^2}} dt. \quad (4)$$

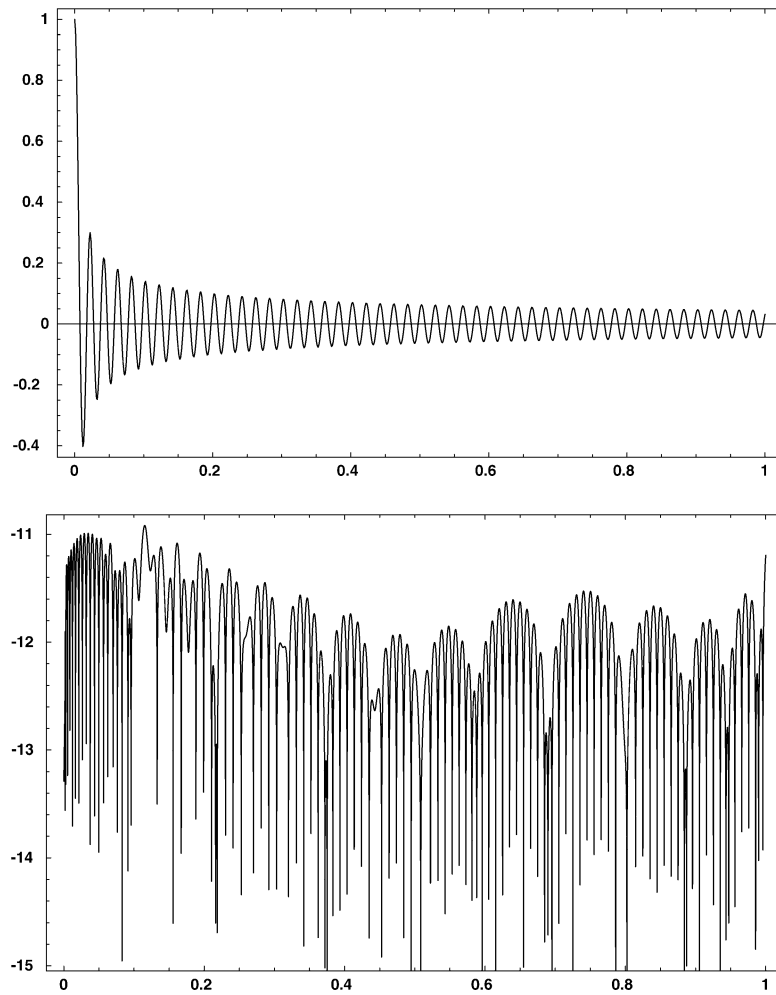


Fig. 1. The function $J_0(100\pi x)$ and the error (in logarithmic scale) of its 28-term approximation via (3).

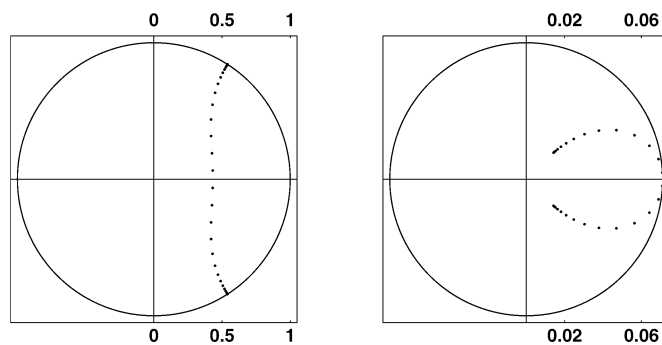


Fig. 2. The complex nodes (left) and weights (right) for the approximation of J_0 in the interval $[0, 100\pi]$.

However, different changes of variables in (4) will result in different contours with no a priori guidance for the choice. Using, for example, $t = \sin(z)$, we have

$$J_0(bx) = \frac{1}{\pi} \int_{-\pi/2}^{\pi/2} e^{ibx \sin(z)} dz, \quad (5)$$

and, with $z = x + iy$, we obtain the steepest descent path as the solution to $\sin x \cosh(y) = \pm 1$, where $|x| \leq \pi/2$ and $y > 0$. The discretization of the integral along this path yields (3) but with more terms than via our method. On the other hand, upon examination of the weights and nodes in Fig. 2, it is clear that their location is not accidental. It appears as if our algorithm selects a contour on which a possible integrand is least oscillatory, since that would reduce the number of necessary nodes.

We note that by optimizing the location of the nodes, we reduce their number to keep it well below the number of terms needed in Fourier expansions or in more general approximations like those discussed in [11]. We do not have a precise estimate for the optimal number of terms but we have observed that it only depends logarithmically on the parameter b and on the accuracy.

We have obtained similar results for a great variety of functions. The functions may be oscillatory, periodic, nonperiodic, or singular. For a given accuracy, we have developed algorithms to obtain the approximation with optimal or nearly optimal number of nodes and weights.

These examples motivate us to formulate the following approximation problem. Given the accuracy $\varepsilon > 0$, for a smooth function $f(x)$ find the minimal (or nearly minimal) number of complex weights w_m and complex nodes e^{t_m} such that

$$\left| f(x) - \sum_{m=1}^M w_m e^{t_m x} \right| \leq \varepsilon \quad \forall x \in [0, 1]. \quad (6)$$

For functions singular at $x = 0$, we formulate (6) on the interval $[\delta, 1]$, where $\delta > 0$ is a small parameter. Depending on the function and/or problem under consideration, we may measure the approximation error in (6) in a different way, e.g., we may use relative error.

As in our paper [11], we reformulate the continuous problem (6) as a discrete problem. Namely, given $2N + 1$ values of $f(x)$ on a uniform grid in $[0, 1]$ and a target accuracy $\varepsilon > 0$, we find the minimal number M of complex weights w_m and complex nodes γ_m such that

$$\left| f\left(\frac{k}{2N}\right) - \sum_{m=1}^M w_m \gamma_m^k \right| \leq \varepsilon \quad \forall k, 0 \leq k \leq 2N. \quad (7)$$

The sampling rate $2N$ has to be chosen as to oversample $f(x)$ and guarantee that the function can be accurately reconstructed from its samples. The nodes and weights in (7) depend on ε and N . Once they are obtained, the continuous approximation (6) is defined using the same weights while the exponents are set as

$$t_m = 2N \log \gamma_m,$$

to match the form in (6). The nonlinear problem of finding the nodes and weights in (7) is split into two problems: to obtain the nodes, we solve a singular value problem and find M roots of a polynomial; to obtain the weights, we use the nodes to solve a well-conditioned linear Vandermonde system.

If in (7) we consider the case $\varepsilon = 0$, we would have an *exact* representation of the sequence of samples as a sum of exponentials, the goal of the so-called Prony's method. We discuss the problems encountered in Prony's method in the next section, but we point out here that by avoiding *exact* representations and incorporating an *arbitrary* but fixed accuracy $\varepsilon > 0$, we manage to control the ill-conditioning encountered in solving this problem and we significantly reduce the number of terms needed in the approximation.

Historically Gaspard de Prony (circa 1795) was the first to address the problem of representing sequences by exponential sums. Unfortunately, his method is numerically unstable and numerous modifications were attempted to improve its numerical behavior (see references in the recent survey [13]). We note that the approximation in (6) can sometimes be obtained by optimization strategies. We refer to [13] for a good review of such approaches. We also note that the approach in [27] is a special purpose optimization strategy for computing quadratures as is that in [4,5] for optimizing rational approximations in the Laplace domain resulting in a particular example of (6). Whereas optimization strategies (e.g., the variable projection method) are applicable to a large variety of problems besides (6), our approach to problems in (6) and (7) makes use of the deep analytic and algebraic structure of these problems and yields fast algorithms for their solution.

The approach in this paper has grown from that in [11] where we used properties of bandlimited functions and of Hermitian Toeplitz matrices to construct solutions of (7). Such a construction leads to specific solutions with nodes on the unit circle and positive weights, but not necessarily with the minimal number of terms as, in this case, their number is always constrained by the Nyquist criterion. In this paper we circumvent the constraints of Fourier analysis by allowing both nodes and weights to be complex-valued, significantly reducing the number of terms in the approximation. Our approach is to construct a Hankel matrix using the values of the function or sequence to be approximated, and use properties of its singular value decomposition to determine the location of nodes and weights for a given accuracy. These nodes and weights define a low rank Hankel approximation of the original Hankel matrix with an error controlled by the singular values. As it turns out, most of the weights are smaller than the target accuracy. As we discard the corresponding terms, we obtain a nearly optimal representation for the matrix. In this sense our approach can be understood as a finite dimensional version of the theory of Adamjan, Arov, and Kreĭn (AAK theory), which involves infinite Hankel matrices as a tool for constructing rational approximations [1–3] (for a recent exposition see [25]). We found no other related methods in the literature.

The paper is organized as follows. In the next section we summarize relevant properties of Hankel matrices and then, in Section 3, we formulate and prove a new representation theorem for finite Hankel matrices. We describe the resulting algorithms in Section 4 and provide several examples as well as applications to fast algorithms in the following section.

As it turns out, several important applications require approximation of functions with singularities where the approximation should remain valid over an extremely large relative range. We develop a reduction approach in Section 6 that allows us to overcome the numerical difficulties of this problem by constructing a nearly optimal approximation from one with a relatively large number of terms (but which is easy to generate). We then apply this approach to approximate the function $f(r) = 1/r^\alpha$, $\alpha > 0$ as a linear combination of Gaussians (needed in a variety of applications); the initial approximation is obtained using the trapezoidal rule to discretize an integral representation of $1/r^\alpha$. We prove the necessary estimates in Appendix A.

2. Preliminary considerations: properties of Hankel matrices

Let us summarize properties of complex-valued Hankel matrices. For a vector \mathbf{h} of complex entries $\mathbf{h} = (h_0, h_1, \dots, h_{2N})$, let $\mathbf{H} = \mathbf{H}_{\mathbf{h}}$ be the $N + 1 \times N + 1$ Hankel matrix defined by \mathbf{h} ,

$$\mathbf{H} = \begin{bmatrix} h_0 & h_1 & \dots & h_N \\ h_1 & \dots & \dots & h_{N+1} \\ \vdots & & & \vdots \\ \dots & \dots & \dots & h_{2N-1} \\ h_N & \dots & h_{2N-1} & h_{2N} \end{bmatrix} \quad (8)$$

that is, $\mathbf{H}_{k,n} = h_{k+n}$ for $0 \leq k, n \leq N$.

2.1. Singular value decomposition and con-eigenvalue problem for Hankel matrices

For a matrix H we will consider the so-called con-eigenvalue problem

$$\mathbf{H}\mathbf{u} = \sigma \bar{\mathbf{u}}, \quad (9)$$

where $\mathbf{u} = (u_0, \dots, u_N)$ is a nonzero vector and σ is real and nonnegative. We use the bar notation to indicate complex conjugation. For a Hankel matrix, (9) is equivalent to

$$\sum_{n=0}^N h_{k+n} u_n = \sigma \bar{u}_k \quad \text{for } 0 \leq k \leq N. \quad (10)$$

Following [17, p. 245], for an arbitrary matrix \mathbf{H} and a complex value σ , a solution $\mathbf{u} \neq 0$ of (9) is said to be a con-eigenvector of \mathbf{H} and σ is then its corresponding con-eigenvalue. We can always select a nonnegative σ , the unique representative of all con-eigenvalues of equal modulus. We refer to such a $\sigma \geq 0$ as a *c-eigenvalue*, to its corresponding con-eigenvector \mathbf{u} as a *c-eigenvector*, and we refer to both of them as a *c-eigenpair* of the matrix. The c-eigenvalues are also solutions of an eigenvalue problem,

Proposition 1 [17, Proposition 4.6.6, p. 246]. *Let \mathbf{A} be any square matrix and σ a nonnegative number. Then, σ is a c-eigenvalue of \mathbf{A} if and only if σ^2 is an eigenvalue of $\bar{\mathbf{A}}\mathbf{A}$.*

Since Hankel matrices are symmetric, $\mathbf{H} = \mathbf{H}^t$, an orthogonal basis of c-eigenvectors can be obtained from Takagi's factorization [17, p. 204] which asserts the existence of a unitary matrix \mathbf{U} and a real nonnegative diagonal matrix $\Sigma = \text{diag}(\sigma_0, \dots, \sigma_N)$, such that

$$\mathbf{H} = \bar{\mathbf{U}}\Sigma\bar{\mathbf{U}}^t = \bar{\mathbf{U}}\Sigma\mathbf{U}^*. \quad (11)$$

This factorization can also be viewed as a singular value decomposition of \mathbf{H} , where the right singular vectors are the complex conjugates of the left singular vectors. We note that (11) is valid regardless of the multiplicity of each singular value and that, for Hankel matrices, the c-eigenvalues coincide with the singular values; we will refer to them in both ways depending on the context.

2.2. Fast application of Hankel matrices

For any vector $\mathbf{x} = (x_0, \dots, x_N)$ denote by \mathbf{P}_x the polynomial $\mathbf{P}_x(z) = \sum_{k \geq 0} x_k z^k$ of degree at most N . We want to compute the vector $\mathbf{H}\mathbf{x}$, where \mathbf{H} is the Hankel matrix defined by the vector \mathbf{h} in \mathbb{C}^{2N+1} . Let L be an integer, $L \geq 2N + 1$ and $\alpha = e^{i2\pi/L}$ a root of unity. We write

$$h_r = \frac{1}{L} \sum_{l=0}^{L-1} \mathbf{P}_h(\alpha^{-l}) \alpha^{rl}, \tag{12}$$

so that for all entries we have

$$(\mathbf{H}\mathbf{x})_k = \frac{1}{L} \sum_{l=0}^{L-1} \mathbf{P}_h(\alpha^{-l}) \mathbf{P}_x(\alpha^l) \alpha^{lk}. \tag{13}$$

This expression can be cast in terms of the discrete Fourier transform (DFT) so that the fast Fourier transform (FFT) provides a fast algorithm to apply Hankel matrices.

2.3. Prony’s method

Let us connect our formulation with the so-called Prony’s method. Let $\mathbf{H} = \mathbf{H}_h$ be a singular Hankel matrix and choose a vector \mathbf{q} in the nullspace of \mathbf{H} . Without loss of generality, we set its last nonzero coordinate to -1 so that $\mathbf{q} = (q_0, \dots, q_{\tilde{N}-1}, -1, 0, \dots, 0)$, where $\tilde{N} \leq N$. If \mathbf{H} were nonsingular, then we extend the vector \mathbf{h} to a vector $\tilde{\mathbf{h}} = (h_0, \dots, h_{2N}, h_{2N+1}, h_{2N+2})$, where h_{2N+1} is a free parameter and h_{2N+2} is chosen in such a way that $\mathbf{H}_{\tilde{h}}$ is a singular matrix.

The equation $\mathbf{H}\mathbf{q} = \mathbf{0}$ is equivalent to a recurrence relation of length \tilde{N} for the entries of the Hankel matrix

$$h_{k+\tilde{N}} = \sum_{n=0}^{\tilde{N}-1} h_{k+n} q_n, \quad k \geq 0. \tag{14}$$

Such recurrence can be solved as

$$h_k = \sum_{n=1}^{\tilde{N}} w_n \gamma_n^k \quad \text{for all } k, \quad 0 \leq k \leq 2N, \tag{15}$$

where $\{\gamma_1, \dots, \gamma_{\tilde{N}}\}$ (which, for now, we assume to be distinct) are the roots of the polynomial \mathbf{P}_q and where the \tilde{N} coefficients w_n are the solution of the Vandermonde system given by the first \tilde{N} equations of (15). If \mathbf{P}_q has multiple roots, a similar representation holds where w_n are replaced by $p_n(k)$, p_n a polynomial of degree strictly less than the multiplicity of the root. Since we seek numerical representations of the form (15), we will always assume distinct roots. Even if they are not distinct, a numerical approximation with distinct roots is always achievable with, perhaps, a few extra terms.

In conclusion, assuming that \mathbf{P}_q has distinct roots, any sequence \mathbf{h} (of odd or even length) can be represented as in (15), where \tilde{N} is at most $N + 1$. These considerations are the essence of Prony’s method to represent a sequence in the form (15). This construction also points out the numerical difficulties encountered by Prony’s method. First, in most problems of interest, the Hankel matrix \mathbf{H} has a large

numerical nullspace that causes severe numerical problems in obtaining a vector \mathbf{q} . Second, the Vandermonde system to obtain the weights w_n in (15) could be extremely ill-conditioned. As it turns out from our results, extracting the roots γ_n from the polynomial \mathbf{P}_q and solving the resulting Vandermonde system is equivalent to solving (14) with infinite precision.

In our approach we are not interested in the *exact* representation (15) but rather in approximate representations for *arbitrary* but fixed accuracy ε ,

$$\left| h_k - \sum_{m=1}^M w_m \gamma_m^k \right| < \varepsilon, \quad (16)$$

with minimal number of terms M . By letting the approximation depend on the accuracy, we are able not only to avoid the numerical problems we just mentioned but also reduce the number of terms.

3. Representation theorems for finite Hankel matrices

In this section we present two main theoretical results. We show how to represent an arbitrary sequence as a linear combination of exponentials and how to describe this representation as a family of approximations of finite Hankel matrices by a particular class of Hankel matrices of low rank. The error of the approximation is expressed in terms of singular values of the Hankel matrix. In this sense our results are similar to AAK theory of infinite-dimensional Hankel operators, see [1–3] and a more recent exposition in [25].

We need some definitions.

- A *c-eigenpolynomial* of \mathbf{H} is the polynomial $\mathbf{P}_u(z) = \sum_{k=0}^N u_k z^k$, where u_k are the entries of the c -eigenvector \mathbf{u} .
- For any c -eigenvector u of a $(N + 1)$ -dimensional Hankel matrix consider the rational function

$$\mathbf{R}_u(z) = \frac{\mathbf{P}_u(z^{-1})}{\mathbf{P}_u(z)},$$

which has unit modulus on the unit circle. For any integer L , $L > 2N$, we define the auxiliary sequence $\tilde{\mathbf{d}} = (\tilde{d}_0, \dots, \tilde{d}_{L-1})$ by evaluating \mathbf{R}_u on a uniform grid on the unit circle. We set

$$\tilde{d}_k = \lim_{z \rightarrow \alpha^k} \mathbf{R}_u(z) \quad \text{for } 0 \leq k < L, \quad (17)$$

where $\alpha = e^{\frac{2\pi i}{L}}$. The periodic sequence $\mathbf{d}^{(L)}$ of entries

$$d_k^{(L)} = \frac{1}{L} \sum_{l=0}^{L-1} \tilde{d}_l \alpha^{lk} \quad \text{for all } k \geq 0, \quad (18)$$

describes the error in our constructions.

We prove

Theorem 2. Let $\{\sigma, \mathbf{u}\}$ be any c -eigenpair of the $(N + 1)$ -dimensional Hankel matrix \mathbf{H} defined by the complex-valued vector $\mathbf{h} = (h_0, \dots, h_{2N})$. Assume that the c -eigenpolynomial $\mathbf{P}_{\mathbf{u}}$ has N distinct roots $\{\gamma_1, \dots, \gamma_N\}$ and choose $L > 2N$. Then, there exists a unique vector (w_1, \dots, w_N) such that

$$h_k = \sum_{n=1}^N w_n \gamma_n^k + \sigma d_k^{(L)} \quad \text{for all } k, 0 \leq k \leq 2N, \quad (19)$$

where $d_k^{(L)}$ is the sequence of unit l^2 norm in \mathbb{C}^L defined in (18).

A similar theorem can be formulated in terms of Hankel matrices. Let us write the approximation sequence as

$$a_k = \sum_{n=1}^N w_n \gamma_n^k, \quad 0 \leq k \leq 2N \quad (20)$$

and denote as $\|\cdot\|$ the matrix 2-norm.

Theorem 3. With the assumptions of Theorem 2, let $\mathbf{H}_{\mathbf{d}}$ and $\mathbf{H}_{\mathbf{a}}$ be the Hankel matrices defined by the vector $\mathbf{d} = (d_0^{(L)}, \dots, d_{2N}^{(L)})$ in (18) and the vector $\mathbf{a} = (a_0, \dots, a_{2N})$ in (20). Then

(1) The Hankel matrix \mathbf{H} defined by the vector \mathbf{h} satisfies

$$\mathbf{H} = \mathbf{H}_{\mathbf{a}} + \sigma \mathbf{H}_{\mathbf{d}}. \quad (21)$$

(2) The Hankel matrix $\mathbf{H}_{\mathbf{d}}$ has unitary 2-norm,

$$\|\mathbf{H}_{\mathbf{d}}\| = 1. \quad (22)$$

(3) The relative error of approximating the Hankel matrix \mathbf{H} by the Hankel matrix $\mathbf{H}_{\mathbf{a}}$ is

$$\frac{\|\mathbf{H} - \mathbf{H}_{\mathbf{a}}\|}{\|\mathbf{H}\|} = \frac{\sigma}{\sigma_0},$$

where σ_0 is the largest singular value of \mathbf{H} .

Remark 4. Theorem 2 yields a different representation for each $L > 2N$ even though γ_n and σ remain the same. That is, for the same set of nodes we have different choices for the weights. The theorem implies that we can obtain the weights $w = (w_1, \dots, w_N)$ as the unique solution of the Vandermonde system

$$h_k - \sigma d_k^{(L)} = \sum_{n=1}^N w_n \gamma_n^k \quad \text{for } 0 \leq k < N. \quad (23)$$

Since the last equation is also valid for $N \leq k \leq 2N$, it follows that the least squares solution (ρ_1, \dots, ρ_N) to the overdetermined problem

$$h_k = \sum_{n=1}^N \rho_n \gamma_n^k \quad \text{for } 0 \leq k \leq 2N, \quad (24)$$

has error with l^2 -norm less than σ .

Remark 5. The assumption that the c-eigenpolynomial of \mathbf{u} has N distinct roots $\{\gamma_1, \dots, \gamma_N\}$ can be relaxed. As explained in Section 2.3, we ask for distinct roots to obtain a sum of exponentials with constant coefficients. Nevertheless, zero could be a multiple root and the representation remains valid except for the first term h_0 . Similarly, the c-eigenpolynomial may have less than N roots, yielding a shorter sum in (19).

Remark 6. Theorems 2 and 3 may be viewed as a finite-dimensional analogue of AAK theory for infinite-dimensional Hankel operators [1–3]. Note that we prove these theorems without any restrictions on the Hankel matrices. However, a practical use of the results requires fast decay of their singular values. In this paper we do not attempt to characterize conditions leading to this property but rather explore some applications of these representations. In this regard we note that in potential signal processing applications no singular value may be very small, a fact that indicates the level of noise in the signal.

Proof of Theorem 2. We will show that the sequence h_k in (19) is the explicit solution of a nonhomogeneous linear recurrence of length $N + 1$. Such a solution can be expressed as the sum of a solution of the homogeneous recurrence (the exponential sum) and a particular solution (the sequence $\sigma d_k^{(L)}$).

We extend the definition of the c-eigenvector \mathbf{u} to a periodic sequence of period L , where we set $u_k = 0$ for $N < k < L$, and use this extended sequence to formulate the following problem. Find a sequence x_k that is the unique solution of

$$\sum_{n=0}^N x_{k+n} u_n = \sigma \bar{u}_k \quad \text{for } k \geq 0, \tag{25}$$

satisfying $x_k = h_k$ for $0 \leq k \leq N - 1$. Such a sequence x_k solves a linear recurrence equation with constant coefficients and N initial conditions. Since we are assuming that $\mathbf{P}_u(z)$ has N distinct roots, we have $u_N \neq 0$ and thus (25) is equivalent to

$$x_{N+k} = - \sum_{n=0}^{N-1} x_{k+n} \frac{u_n}{u_N} + \sigma \frac{\bar{u}_k}{u_N} \quad \text{for } k \geq 0,$$

where x_0, \dots, x_{N-1} are given. If $x_k^{(p)}$ is a particular solution of (25), any other solution can be written as

$$x_k = \sum_{n=1}^N w_n \gamma_n^k + x_k^{(p)},$$

where the w_n are uniquely determined by the initial values. In fact, they are the solution of the square Vandermonde system

$$\sum_{n=1}^N w_n \gamma_n^k = h_k - x_k^{(p)} \quad \text{for } 0 \leq k \leq N - 1.$$

To prove the theorem, we only need to show that $\sigma d_k^{(L)}$, for $d_k^{(L)}$ defined in (18), is a particular solution of (25), or because of the periodicity of \mathbf{u} and $\mathbf{d}^{(L)}$, show that

$$\sum_{n=0}^N d_{k+n}^{(L)} u_n = \bar{u}_k \quad \text{for } 0 \leq k \leq L - 1. \tag{26}$$

Using (18) we expand the left-hand side of (26)

$$\sum_{n=0}^N d_{k+n}^{(L)} u_n = \frac{1}{L} \sum_{l=0}^{L-1} \tilde{d}_l \alpha^{kl} \sum_{n=0}^N u_n \alpha^{nl} = \frac{1}{L} \sum_{l=0}^{L-1} \tilde{d}_l \mathbf{P}_{\mathbf{u}}(\alpha^l) \alpha^{kl},$$

and, due to (17), the last term equals

$$\frac{1}{L} \sum_{l=0}^{L-1} \mathbf{P}_{\tilde{\mathbf{u}}}(\alpha^{-l}) \alpha^{kl} = \tilde{u}_k.$$

Finally, since $|\tilde{d}_k| = 1$ for all k , the l^2 norm of $\mathbf{d}^{(L)}$ equals 1. \square

Next, we prove Theorem 3.

Proof. Part (1) is a direct consequence of (19), while part (3) follows from the first two. For part (2), (26) implies

$$\mathbf{H}_{\mathbf{d}} \mathbf{u} = \tilde{\mathbf{u}},$$

and with the notation $\|\cdot\|$ for both the matrix 2-norm and the vector l^2 -norm, we derive $\|\mathbf{H}_{\mathbf{d}}\| \geq \frac{\|\mathbf{H}_{\mathbf{d}} \mathbf{u}\|}{\|\mathbf{u}\|} = 1$; thus, the norm is at least one. To see that it is at most one, let $\mathbf{v} \in \mathbb{C}^{N+1}$ and use (13) and (18) to write for $0 \leq k \leq N$,

$$(\mathbf{H}_{\mathbf{d}} \mathbf{v})_k = \frac{1}{\sqrt{L}} \sum_{l=0}^{L-1} \left(\frac{\tilde{d}_l \mathbf{P}_{\mathbf{v}}(\alpha^l)}{\sqrt{L}} \right) \alpha^{kl}.$$

The right-hand side of the last equation is well defined for $0 \leq k \leq L-1$, and corresponds to the DFT of the vector $\frac{\tilde{d}_l \mathbf{P}_{\mathbf{v}}(\alpha^l)}{\sqrt{L}}$. Since the DFT is unitary and $|\tilde{d}_l| = 1$, we obtain

$$\|\mathbf{H}_{\mathbf{d}} \mathbf{v}\|^2 \leq \left\| \frac{\tilde{d}_l \mathbf{P}_{\mathbf{v}}(\alpha^l)}{\sqrt{L}} \right\|^2 = \|\mathbf{v}\|^2.$$

The last inequality holds for any vector \mathbf{v} , implying that $\|\mathbf{H}_{\mathbf{d}}\| \leq 1$. \square

3.1. Number of nodes and decay of the singular values

Although Theorem 2 holds for any singular value σ , we plan to use (20) as an approximation of the given sequence h_k with absolute error at most σ . For this reason we are interested only in small singular values. Moreover, we discard many terms in the exponential sum (20) because we have observed that most of them have weights with values below σ . We have already encountered this situation in [11], where the number of terms in the approximation is controlled by the index of the singular value. If we label the singular values in decreasing order,

$$\sigma_0 \geq \sigma_1 \geq \dots \geq \sigma_N,$$

and choose the index M , $M \leq N$, in such a way that σ_M is close to the accuracy sought, we have observed that only M weights in (20) are larger than σ_M . In Fig. 3 we display the locations of all the roots of the c-eigenpolynomial corresponding to $\sigma_{28} \sim 10^{-10}$ using our previous example with the Bessel function

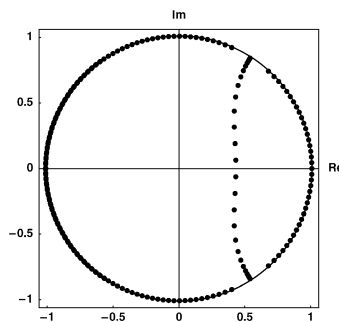


Fig. 3. Locations of all roots of the c-eigenpolynomial corresponding to the singular value σ_{28} in the approximation of J_0 in $[0, 100\pi]$. In practice, we only use the 28 roots inside the unit disk.

$J_0(x)$ in the interval $[0, 100\pi]$. The 28 significant weights (see Fig. 2) are associated with the nodes inside the unit disk. We note that the nodes corresponding to the discarded terms are located outside but very close to the unit circle. The error of the 28-terms approximation is displayed in Fig. 1.

By keeping only the terms with significant weights, the singular value index M provides a M -term approximation of the sequence h_k with error of the order of σ_M . This behavior matches that of indices of the singular values in AAK theory, where the M th singular value of the Hankel operator equals the distance from that operator to the set of Hankel operators of rank at most M .

Currently we do not have a characterization of the conditions under which finite Hankel matrices may satisfy the results of the infinite theory. We only note that assuming fast decay of the singular values and that $N - M$ terms have small weights in (19), the approximation $b_k = \sum_{m=1}^M w_m \gamma_m^k$ has the optimal number of terms. Indeed, let \mathbf{H}_b be the corresponding Hankel matrix for \mathbf{b} . Since \mathbf{H}_b has rank M , we have

$$\sigma_M \leq \|\mathbf{H} - \mathbf{H}_b\| < \sigma_M + \delta \quad (27)$$

for some $\delta > 0$. Under the assumptions of $N - M$ small weights and of fast decay of the singular values, it is reasonable to expect δ small enough so that $\sigma_M + \delta \leq \sigma_{M-1}$, therefore preventing an approximation with a shorter sum.

The practical value of our approximation depends then on the fast decay of the singular values of the Hankel matrix \mathbf{H}_h . Fortunately, in problems of interest, we have observed such decay. In fact, in many problems the decay is exponential and we obtain approximations where the number of terms increases only logarithmically with the accuracy. In Fig. 4 we illustrate this property for the Bessel function $J_0(x)$.

3.2. Computation of weights

In our paper [11] weights are computed via a fast algorithm based on implementation of the relations (19) for nodes on the unit circle. We use the fact that the solution of a Vandermonde system is obtained as polynomial evaluation on the Vandermonde nodes. The coefficients of the polynomial are computed using the FFT and the evaluation on the nodes is computed via the unequally spaced FFT (USFFT) (see, e.g., [7,12]) because the nodes are on the unit circle. We also showed in [11] that even though Vandermonde systems can be arbitrarily ill-conditioned, the approximation problem on the unit circle is well posed due to the particular location of the nodes and the specific right-hand sides.

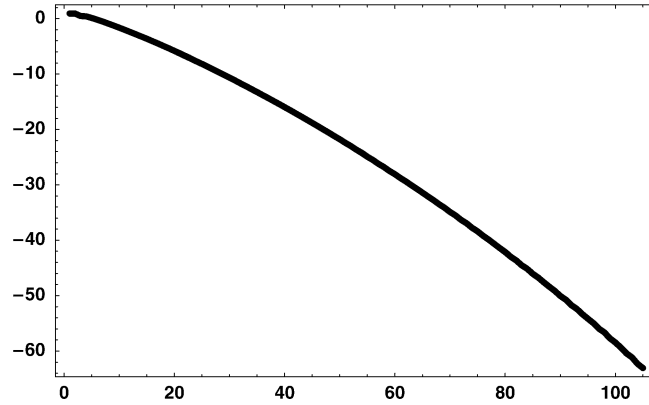


Fig. 4. Example of exponential decay of singular values (we display log of singular values as a function of their index) in the approximation of $J_0(100\pi x)$ in $[0, 1]$.

In this paper nodes are typically inside the unit disk, thus preventing the direct use of the USFFT. Nevertheless, since the number of significant terms is small, to solve the Vandermonde system (23) both polynomial evaluation or the least squares formulation (24) are efficient options. We choose the particular approach depending on the location of nodes or additional information about the problem.

3.3. Trigonometric moments and Toeplitz matrices

In [11] we have shown how to approximate nonperiodic bandlimited functions as linear combinations of exponentials with imaginary exponents, that is, with nodes on the unit circle. In that paper, samples of the function to be approximated (which can be thought as trigonometric moments of a positive measure) are used to build a Hermitian Toeplitz matrix whose eigenpolynomials happen to have roots on the unit circle. Even though most of the results in [11] are based on the particular properties of bandlimited functions, and as such, cannot be directly obtained by the general method of this paper, some results in [11] are immediate consequences of the general approach presented here. As an example, consider \mathbf{T} a Toeplitz Hermitian matrix and $\{\sigma, \mathbf{u}\}$ an eigenpair of \mathbf{T} ; we assume that the entries of \mathbf{u} satisfy $u_{N-k} = \bar{u}_k$, $0 \leq k \leq N$ and that the eigenpolynomial $\mathbf{P}_{\mathbf{u}}$ has distinct roots. Let \mathbf{J} be the matrix with ones in the antidiagonal. Then $\mathbf{H} = \mathbf{J}\mathbf{T}$ is a Hankel matrix and $\{\sigma, \mathbf{u}\}$ is a c-eigenpair of \mathbf{H} ; since the eigenpolynomial of \mathbf{u} satisfies $\mathbf{P}_{\bar{\mathbf{u}}}(z^{-1}) = z^{-N}\mathbf{P}_{\mathbf{u}}(z)$, the entries of the sequence $\tilde{\mathbf{d}}$ in (17) satisfy

$$\tilde{d}_k = e^{-\frac{2\pi kiN}{L}}$$

and so the error sequence $d_k^{(L)}$ in (19) has zero entries except at $k = N$, which coincides with our previous description of the error for a Toeplitz Hermitian matrix [11, Theorem 4.1 and Corollary 4.1].

4. A new algorithm for approximations by sum of exponentials

We now describe how to compute the approximation described in (7). Given the target accuracy ε and $2N + 1$ samples

$$h_k = f\left(\frac{k}{2N}\right), \quad 0 \leq k \leq 2N \quad (28)$$

of the function to be approximated in the interval $[0, 1]$, our goal is to find an optimal (minimal) number of nodes γ_m and weights w_m such that

$$\left| h_k - \sum_{m=1}^M w_m \gamma_m^k \right| < \varepsilon \quad \forall k, 0 \leq k \leq 2N. \quad (29)$$

If the function $f(x)$ is properly oversampled, we also obtain the continuous approximation (7) of $f(x)$ over the interval $[0, b]$.

Let us describe the steps of the algorithm to obtain an approximation of the function f with accuracy ε .

- (1) Sample the function f as in (28) by choosing appropriate N to achieve the necessary oversampling. Using those samples define the corresponding $N + 1 \times N + 1$ Hankel matrix $\mathbf{H}_{kl} = h_{k+l}$.
- (2) Find a c -eigenpair $\{\sigma, \mathbf{u}\}$, $\mathbf{H}\mathbf{u} = \sigma\mathbf{u}$, with the c -eigenvalue σ close to the target accuracy ε . We use an algorithm that recovers the c -eigenpairs starting from the largest c -eigenvalue up to the one we seek. Because we are interested in functions which exhibit fast decay of their c -eigenvalues, only a small number of c -eigenpairs are computed. We label the computed c -eigenvalues in decreasing order $\sigma_0 \geq \sigma_1 \geq \dots \geq \sigma_M$, where $M \ll N$.
- (3) If the c -eigenvector u has entries (u_0, \dots, u_N) , we find M roots of the c -eigenpolynomial $\sum_{k=0}^N u_k z^k$ in the “significant” region. We denote these roots $\gamma_1, \dots, \gamma_M$ and refer to them as c -eigenroots. In finding c -eigenroots corresponding to the significant weights, we typically use a priori information on their location, such as being inside the unit disk, being close to the unit circle, located on a curve, etc.
- (3) We obtain the M weights w_m by solving the Vandermonde system (23) or the overdetermined Vandermonde system (24).

Remark 7. If the approximation problem does not involve an explicit function but the goal is to obtain the approximation (29) of a given sequence h_k , the same algorithm is used but without the first step.

5. Examples

Let us describe how to apply the algorithm in Section 4 to obtain the approximation (3) of the Bessel function $J_0(bx)$ in $[0, 1]$, where $b = 100\pi$ and $\varepsilon = 10^{-10}$. The function and the approximation error are displayed in Fig. 1. Our choice of $N = 214$ includes 16 extra samples to improve the accuracy at the edges of the interval. We compute the c -eigenpairs using the power method and the fact that c -eigenvectors are orthogonal; see (11) and recall that c -eigenvalues coincide with the singular values of \mathbf{H} . In this example, starting with $\sigma_0 = 8.34$, we compute a total of 29 singular values until we reach the accuracy ε . In fact we obtain $\sigma_{27} = 2.295 \times 10^{-10}$ and $\sigma_{28} = 7.527 \times 10^{-11}$; the decay of the first 110 singular values is captured in Fig. 4. To obtain the nodes, we now need to find 28 particular roots of the c -eigenpolynomial. In order to show that these roots belong to a well-defined region, we actually compute all 214 roots and display them in Fig. 3. Two distinctive regions can be seen. The first region is outside but very close to the unit circle and the second is inside the unit disk, with 28 roots accumulating

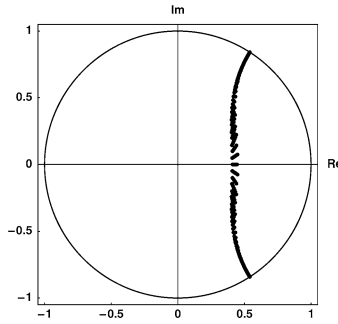


Fig. 5. Nodes corresponding to singular values in the range $[4.7 \times 10^{-15}, 6.7 \times 10^{-9}]$ for the approximation of $J_0(100\pi x)$.

at e^i and e^{-i} . It is instructive to observe how roots in the first region stay some distance away from these accumulation points. As we have mentioned in the Introduction, this accumulation can be expected from the asymptotics of the Bessel function. More important from a computational perspective is that the nodes slowly change their locations as we modify either the approximation interval (parametrized by the constant b) or the accuracy ε (parametrized by the singular values). In this way, computation of roots can be performed efficiently by, if necessary, obtaining first the nodes for a small b and using them as starting points in Newton’s method. To illustrate this property, in Fig. 5 we display the nodes for a range of singular values varying from 6.7×10^{-9} to 4.7×10^{-15} .

As we noted for Fig. 2, the locations of nodes and weights suggest the existence of some integral representation of J_0 on a contour in the complex plane where the integrand is least oscillatory; integration over such contour yields an efficient discretization that would correspond to the output of our algorithm.

The final approximation (6) exhibits an interesting property that we also have observed for other oscillatory functions. Suppose that we would like to obtain a decreasing function (an envelope) that touches each of the local maxima of the Bessel function and, similarly, a increasing function going through each of the local minima. The approximation (6) provides such functions in a natural way. Estimating the absolute value of an exponential sum, we define its positive envelope $\text{env}(x)$ as

$$\left| \sum_{m=1}^M w_m e^{t_m x} \right| \leq \sum_{m=1}^M |w_m| e^{\text{Re}(t_m)x} = \text{env}(x),$$

and its *negative envelope* as $-\text{env}(x)$. In Fig. 6 we display the Bessel function $J_0(100\pi x)$ together with its envelopes. We note that we are not aware of any other simple method to obtain such envelopes.

5.1. The Dirichlet kernel

Another representative example is the periodic Dirichlet kernel,

$$D_n(x) = \frac{1}{N} \sum_{k=-n}^n e^{2\pi i k x} = \frac{\sin N\pi x}{N \sin \pi x}, \tag{30}$$

where $N = 2n + 1$. We would like to construct an approximation (6) of D_n on the interval $[0, 1]$. Since D_n is an even function about $1/2$ and it approaches 1 near $x = 1$ (see Fig. 8), decaying exponentials are not sufficient to capture this behavior. Therefore, the approximation must have nodes both inside and

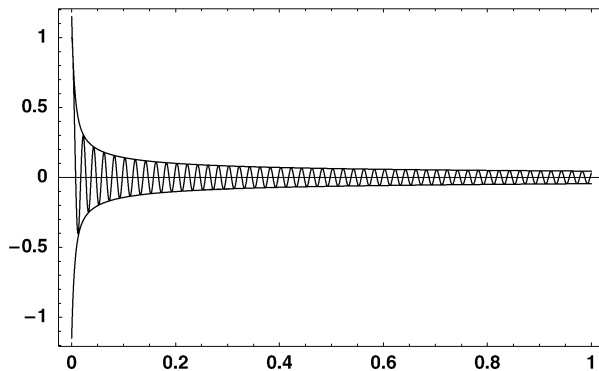


Fig. 6. The Bessel function $J_0(100\pi x)$ together with its envelope functions.

outside the unit circle. In this case the Vandermonde matrix for computing the weights is extremely ill conditioned. As a way to avoid this difficulty, we reduce the problem to that of approximation of an auxiliary function with a proper decay.

Using the partial fraction expansion of the cosecant

$$\sum_{k \in \mathbb{Z}} \frac{(-1)^k}{x+k} = \frac{\pi}{\sin(\pi x)},$$

we have

$$D_n(x) = \frac{\sin(N\pi x)}{N\pi} \sum_{k \in \mathbb{Z}} \frac{(-1)^k}{x+k} = \sum_{k \in \mathbb{Z}} \frac{\sin(N\pi(x+k))}{N\pi(x+k)}.$$

Motivated by this identity, we introduce the function

$$G_n(x) = \frac{\sin(N\pi x)}{N\pi} \sum_{k \geq 0} \frac{(-1)^k}{x+k} = \sum_{k \geq 0} \frac{\sin(N\pi(x+k))}{N\pi(x+k)},$$

and observe that

$$D_n(x) = G_n(x) + G_n(1-x). \quad (31)$$

We then solve the approximation problem for G_n in $[0, 1]$,

$$\left| G_n(x) - \sum_{m=1}^M \rho_m e^{t_m x} \right| \leq \varepsilon, \quad (32)$$

where weights and nodes are complex and $|e^{t_m}| < 1$. In Fig. 7 we display the location of the nodes and weights where $n = 50$ and $\varepsilon = 10^{-8}$. The singular values of the corresponding Hankel matrix are decaying exponentially, similar to the decay in Fig. 4. The number of terms grows logarithmically with the accuracy and with n , $M = \mathcal{O}(\log n) + \mathcal{O}(\log \varepsilon)$.

Using (31) and (32), we obtain the approximation for the Dirichlet kernel,

$$\left| D_n(x) - \sum_{m=1}^M \rho_m e^{t_m x} - \sum_{m=1}^M \rho_m e^{t_m(1-x)} \right| \leq 2\varepsilon. \quad (33)$$

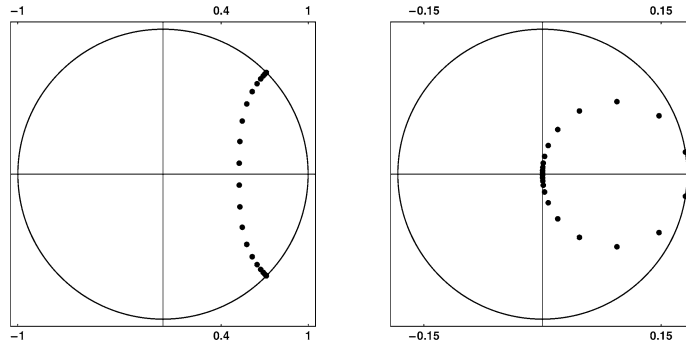


Fig. 7. The 22 nodes (left) and weights (right) for the approximation of the auxiliary function G_{50} in $[0, 1]$.

We note that $|e^{-t_m}| > 1$ and, thus, the final approximation of D_n has nodes both inside and outside of the unit disk. In Fig. 8 we display the Dirichlet kernel D_{50} and the error of the approximation with 44 terms given by this construction. For D_{200} we need 50 terms.

5.2. The kernels $\log \sin^2(\pi x)$ and $\cot(\pi x)$

Let us consider two examples of important kernels in harmonic analysis. The function $\log \sin^2(\pi x)$ is the kernel of the Neumann to Dirichlet map on the unit circle for functions harmonic outside the unit disk whereas $\cot(\pi x)$ is the Hilbert kernel for functions on the unit circle. We note that the Hilbert kernel represents a singular operator.

We first find identities similar to (31). Using the reflection formula for the gamma function,

$$\Gamma(x)\Gamma(1-x) = \frac{\pi}{\sin(\pi x)}, \tag{34}$$

we obtain

$$\log \Gamma(x) + \log \Gamma(1-x) = \log \pi - \frac{1}{2} \log \sin^2 \pi x. \tag{35}$$

For the cotangent we use the reflection formula for the digamma function, $\psi(x) = (\ln \Gamma(x))' = \frac{\Gamma'(x)}{\Gamma(x)}$,

$$\psi(x) - \psi(1-x) = -\pi \cot \pi x. \tag{36}$$

We now solve the approximation problems on $[\delta, 1)$,

$$\left| \log \Gamma(x) - \sum_{m=1}^M \rho_m^0 e^{-t_m^0 x} \right| \leq \varepsilon,$$

and

$$\left| -\psi(x) - \sum_{m=1}^M \rho_m^1 e^{-t_m^1 x} \right| \leq \varepsilon,$$

where t_m^0 and t_m^1 are real and $\delta > 0$ is a small number. We then obtain the final approximations as

$$\left| \frac{1}{2} \log \sin^2(\pi x) - \log \pi + \sum_{m=1}^M \rho_m^0 e^{-t_m^0 x} + \sum_{m=1}^M \rho_m^0 e^{-t_m^0(1-x)} \right| \leq 2\varepsilon, \tag{37}$$

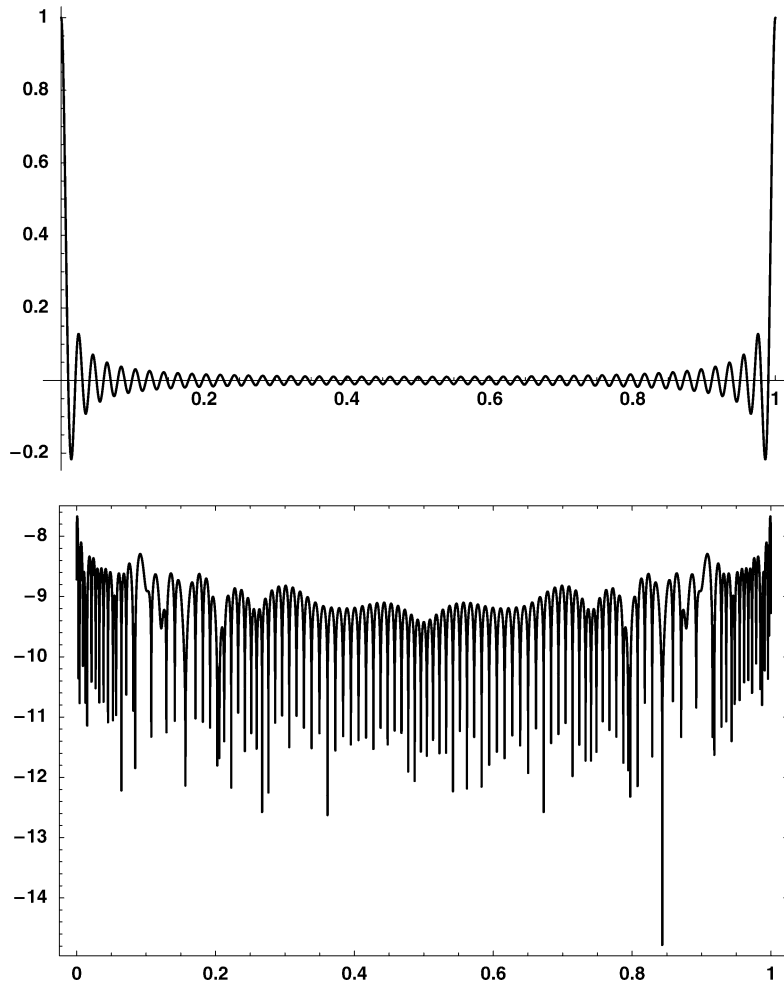


Fig. 8. Dirichlet kernel D_{50} (top) and the error (in logarithmic scale) of its 44-term approximation via (33).

and

$$\left| \pi \cot \pi x - \sum_{m=1}^M \rho_m^1 e^{-t_m^1 x} + \sum_{m=1}^M \rho_m^1 e^{-t_m^1 (1-x)} \right| \leq 2\varepsilon. \quad (38)$$

5.3. Fast evaluation of one-dimensional kernels

Let us consider computing

$$g(x) = \int_0^1 K(x-y) f(y) dy, \quad (39)$$

at points $\{x_n\}_{n=1}^N$, $x_n \in [0, 1]$. In practice, we need to compute the sum

$$g(x_n) = \sum_{l=1}^L K(x_n - y_l) f(y_l), \tag{40}$$

where we assume that the discretization of the integral (39) has already been performed by some appropriate quadrature and we include the quadrature weights in $f(y_l)$.

The direct computation of (40) requires $N \cdot L$ operations. If we first obtain an M -term exponential approximation of the kernel, an elegant algorithm [28] computes the sum with accuracy ε in $\mathcal{O}(2M \cdot (L + N))$ operations, where M is the number of terms in

$$\left| K(s) - \sum_{m=1}^M \rho_m e^{t_m s} \right| \leq \varepsilon \quad \text{for } s \in [0, 1] \tag{41}$$

assuming that the kernel K is an even function, $K(-s) = K(s)$. Alternatively, we also need an exponential approximation of the kernel on the interval $[-1, 0]$ and, in such case, the number of operations becomes $\mathcal{O}((M^+ + M^-) \cdot (L + N))$, where M^+ and M^- are the number of terms for the approximation on $[0, 1]$ and $[-1, 0]$.

For a simplified version of the algorithm, split the sum (40) as

$$g(x_n) = \sum_{0 \leq y_l \leq x_n} K(x_n - y_l) f(y_l) + \sum_{x_n < y_l \leq 1} K(x_n - y_l) f(y_l), \tag{42}$$

and compute each term separately. Using (41), we approximate the first term in (42) as

$$\sum_{m=1}^M w_m q_{n,m}, \quad \text{where } q_{n,m} = \sum_{0 \leq y_l \leq x_n} e^{t_m(x_n - y_l)} f(y_l)$$

and similarly for the second term in the sum.

Following [28], we observe that

$$q_{n+1,m} = e^{t_m(x_{n+1} - x_n)} \sum_{0 \leq y_l \leq x_n} e^{t_m(x_n - y_l)} f(y_l) + \sum_{x_n < y_l \leq x_{n+1}} e^{t_m(x_{n+1} - y_l)} f(y_l),$$

and, thus, $q_{n,m}$ is computed via the recursion

$$q_{n+1,m} = e^{t_m(x_{n+1} - x_n)} q_{n,m} + \sum_{x_n < y_l \leq x_{n+1}} e^{t_m(x_{n+1} - y_l)} f(y_l).$$

As long as $\text{Re}(t_m) \leq 0$, we have a stable recursion which takes $\mathcal{O}(N + L)$ operations to evaluate. Since we need to compute $q_{n,m}$ for $m = 1, \dots, M$ for both terms in (42), the resulting computational cost is $\mathcal{O}(2M \cdot (L + N))$.

If the kernel has a singularity at $x = y$, the splitting in (42) should be done as to maintain an appropriate distance from the singularity. This is, in fact, how the algorithm was originally designed in [28]. In that paper the approximation for the nonsingular Dirichlet kernel (30) is constructed by approximating $1/\sin(\pi x)$, an approach that introduces an artificial singularity. Algorithmically such singularity forces an additional term in (42) for the direct evaluation of the kernel near the singularity; this is avoided if we use (41) to approximate the Dirichlet kernel.

6. Reduction of number of terms

The algorithm in Section 4 allow us to find approximations for a large variety of functions but it is not well suited to deal with the extremely large ranges needed in some applications. Also, we would like to have a mechanism to approximate functions that can be expressed in terms of other functions for which we already have exponential sum approximations. Clearly, the nodes and weights for the sum or product of two known approximations are readily available, but their number is suboptimal. Similarly, an accurate but suboptimal expansion may be available, for example as the result of using some quadrature rule or simply applying the discrete Fourier transform of the data to be approximated. We now show how to take advantage of accurate but suboptimal approximations using a general approach on how to reduce (optimize) the number of terms of a given exponential sum. It consists of applying the algorithm of Section 4 to a function which is already a linear combination of exponentials on the interval $[0, 1]$ and taking advantage of some simplifications which hold for this particular class of functions. We obtain a fast algorithm for the following problem. Given

$$f(x) = \sum_{m=1}^{M_0} b_m e^{-\tau_m x}, \quad (43)$$

and $\varepsilon > 0$, let us find a function (of the same form),

$$g(x) = \sum_{m=1}^M w_m e^{-t_m x}, \quad (44)$$

with $M < M_0$ and such that

$$|f(x) - g(x)| \leq \varepsilon \quad \text{for } x \in [0, 1]. \quad (45)$$

Without loss of generality, we assume distinct τ_m and nonzero b_m in (43). Following the algorithm in Section 4, for some appropriate $N \gg M_0$, we construct the Hankel matrix $\mathbf{H} = h_{n+n'}$, $n, n' = 0, \dots, N$, where

$$h_n = f\left(\frac{n}{2N}\right) = \sum_{m=1}^{M_0} b_m e^{-\frac{\tau_m}{2N} n}. \quad (46)$$

Denoting $r_m = e^{-\frac{\tau_m}{2N}}$, $m = 1, \dots, M_0$, we have

$$h_n = \sum_{m=1}^{M_0} b_m r_m^n, \quad (47)$$

and, therefore, a factorization of the Hankel matrix

$$\mathbf{H} = \mathbf{V}\mathbf{B}\mathbf{V}^t, \quad (48)$$

where \mathbf{V} is the $(N+1) \times M_0$ Vandermonde matrix

$$\mathbf{V}_{km} = r_m^k \quad (49)$$

and \mathbf{B} is the diagonal matrix with entries (b_1, \dots, b_{M_0}) . We note that the matrix \mathbf{H} has a large nullspace of dimension $N+1 - M_0$. In fact, the nullspace consists of vectors with coordinates given by the coefficients of the polynomials $\prod_{m=1}^{M_0} (z - r_m) p(z)$, where $p(z)$ is any polynomial of degree at most $N - M_0$.

By excluding the nullspace of \mathbf{H} , which corresponds to zero c-eigenvalues, we now show how to reduce a c-eigenproblem for \mathbf{H} to a c-eigenproblem for an auxiliary matrix of size $M_0 \times M_0$. We also show how to use this approach to effectively compute the nodes and weights in the approximation of h_n .

Consider $\sigma > 0$ and $\mathbf{u} = (u_0, \dots, u_N) \neq 0$, a solution of the c-eigenproblem of \mathbf{H} ,

$$\sum_{n'=0}^N h_{n+n'} u_{n'} = \sigma \bar{u}_n, \quad n = 0, \dots, N. \quad (50)$$

Equation (47) allows us to rewrite (50) as

$$\sum_{m=1}^{M_0} b_m r_m^n \mathbf{P}_{\mathbf{u}}(r_m) = \sigma \bar{u}_n, \quad (51)$$

where $\mathbf{P}_{\mathbf{u}}$ is the c-eigenpolynomial of \mathbf{u} . Multiplying (51) by z^n and summing over the index n , we obtain

$$\sum_{m=1}^{M_0} b_m \frac{1 - (r_m z)^{N+1}}{1 - r_m z} \mathbf{P}_{\mathbf{u}}(r_m) = \sigma \mathbf{P}_{\bar{\mathbf{u}}}(z). \quad (52)$$

Even though the c-eigenpolynomial has degree N , it has a much shorter, rational-like representation suitable to compute its zeros. This representation depends on its values on the given locations r_m . We now obtain those values as solutions of an auxiliary c-eigenproblem.

Let us write the polar decomposition of the coefficients b_m ,

$$b_m = \rho_m e^{i\theta_m} \quad \text{with } \rho_m > 0$$

and denote their square roots as $c_m = \sqrt{\rho_m} e^{i\theta_m/2}$.

Substituting $z = \bar{r}_k$ in (52) and multiplying by \bar{c}_k we obtain

$$\sum_{m=1}^{M_0} \bar{c}_k \frac{1 - (r_m \bar{r}_k)^{N+1}}{1 - r_m \bar{r}_k} c_m^2 \mathbf{P}_{\mathbf{u}}(r_m) = \sigma \overline{c_k \mathbf{P}_{\mathbf{u}}(r_k)}. \quad (53)$$

Introducing the $M_0 \times M_0$ matrix \mathbf{A} ,

$$A_{km} = \bar{c}_k \frac{1 - (r_m \bar{r}_k)^{N+1}}{1 - r_m \bar{r}_k} c_m, \quad (54)$$

and defining the vector \mathbf{v} of coordinates

$$v_k = c_k \mathbf{P}_{\mathbf{u}}(r_k),$$

we rewrite (53) to obtain

$$\mathbf{A}\mathbf{v} = \sigma \bar{\mathbf{v}}. \quad (55)$$

Since $\mathbf{u} \neq 0$, (52) guarantees that not all $\mathbf{P}_{\mathbf{u}}(r_m)$ are zero and thus $\mathbf{v} \neq 0$. We conclude that if $\{\sigma, \mathbf{u}\}$ is a c-eigenpair of \mathbf{H} and $\sigma \neq 0$, then $\{\sigma, \mathbf{v}\}$ is a c-eigenpair of \mathbf{A} . In Proposition 8 we show that the converse result is also true. Thus, instead of solving (50) for a large size matrix, we solve the small size c-eigenvalue problem (55) for an appropriate $\sigma = \sigma_M$ close to the target accuracy ε . We use (52) to describe the c-eigenpolynomial $\mathbf{P}_{\mathbf{u}}$ of the original matrix \mathbf{H} as

$$\mathbf{P}_{\bar{\mathbf{u}}}(z) = \frac{1}{\sigma} \sum_{m=1}^{M_0} c_m \frac{1 - (r_m z)^{N+1}}{1 - r_m z} v_m. \quad (56)$$

Using (56) we find the M zeros in the region of interest, $\mathbf{P}_u(\gamma_m) = 0$, $1 \leq m \leq M$. The final exponents t_m for the reduced approximation (44) are then $t_m = -2N \log \gamma_m$. Finally, we solve for w_m , $1 \leq m \leq M$ using the overdetermined system,

$$h_n = \sum_{m=1}^M w_m \gamma_m^n, \quad n = 0, \dots, 2N. \tag{57}$$

The normal equations of this system are,

$$\sum_{n=0}^{2N} \bar{\gamma}_s^n h_n = \sum_{m=1}^M w_m \sum_{n=0}^{2N} (\gamma_m \bar{\gamma}_s)^n = \sum_{m=1}^M w_m \frac{1 - (\gamma_m \bar{\gamma}_s)^{2N+1}}{1 - \gamma_m \bar{\gamma}_s}. \tag{58}$$

Substituting (47) into (58) we obtain w_m , $1 \leq m \leq M$ as the unique solution of

$$\sum_{m=1}^M \frac{1 - (\gamma_m \bar{\gamma}_s)^{2N+1}}{1 - \gamma_m \bar{\gamma}_s} w_m = \sum_{m=1}^{M_0} \frac{1 - (r_m \bar{\gamma}_s)^{2N+1}}{1 - r_m \bar{\gamma}_s} b_m.$$

We note that the auxiliary $M_0 \times M_0$ matrix \mathbf{A} in (55) is positive definite. In fact, (54) is equivalent to

$$\mathbf{A} = \mathbf{S}^* \mathbf{S} \quad \text{for } \mathbf{S} = \mathbf{V} \mathbf{C}, \tag{59}$$

where \mathbf{C} is the diagonal matrix with entries (c_1, \dots, c_{M_0}) and \mathbf{V} is the rectangular Vandermonde matrix in (49). Thus, for any nonzero vector \mathbf{x} , the inner product $\langle \mathbf{A} \mathbf{x}, \mathbf{x} \rangle = \|\mathbf{V} \mathbf{C} \mathbf{x}\|^2$ is always positive because \mathbf{V} has zero nullspace. Therefore, by [17, Theorem 4.6.11, p. 248], there exist a nonsingular matrix \mathbf{M} and a diagonal matrix \mathbf{D} such that $\mathbf{A} = \mathbf{M} \mathbf{D} \mathbf{M}^{-1}$. The c -eigenvalues of \mathbf{A} are the eigenvalues of $\bar{\mathbf{A}} \mathbf{A}$ (see Proposition 1). Note that for \mathbf{A} with complex entries, the M_0 c -eigenvalues of \mathbf{A} (which are real and positive) do not need to coincide with their singular values.

Proposition 8. *Let \mathbf{H} be a $N + 1 \times N + 1$ Hankel matrix defined by the vector (47) and \mathbf{A} the $M_0 \times M_0$ positive definite matrix in (54). Consider any c -eigenpair of \mathbf{A} ,*

$$\mathbf{A} \mathbf{v} = \sigma \bar{\mathbf{v}},$$

and define the vector \mathbf{u} of entries

$$u_k = \frac{1}{\sigma} \overline{\sum_{m=1}^{M_0} c_m v_m r_m^k}, \tag{60}$$

where v_m are the entries of the c -eigenvector \mathbf{v} . Then

- (1) The value σ and the vector \mathbf{u} are a c -eigenpair of \mathbf{H} , $\mathbf{H} \mathbf{u} = \sigma \bar{\mathbf{u}}$.
- (2) The polynomial $\mathbf{P}_{\bar{\mathbf{u}}}$, with coefficients that are the entries of $\bar{\mathbf{u}}$, satisfies the identity (56).
- (3) The c -eigenpolynomial $\mathbf{P}_{\mathbf{u}}$ at any of the original nodes r_m has values

$$\mathbf{P}_{\mathbf{u}}(r_m) = \frac{v_m}{c_m} \quad \text{for } 1 \leq m \leq M_0.$$

Proof. With \mathbf{S} defined as in (59), we have $\mathbf{H} = \mathbf{S} \mathbf{S}^t$, $\mathbf{A} = \mathbf{S}^* \mathbf{S}$, and $\mathbf{u} \frac{\bar{\mathbf{S}} \mathbf{v}}{\sigma}$. Then,

$$\mathbf{H} \mathbf{u} = \frac{\overline{\mathbf{S} \mathbf{S}^* \mathbf{S} \mathbf{v}}}{\sigma} = \frac{\overline{\mathbf{S} \mathbf{A} \mathbf{v}}}{\sigma} = \mathbf{S} \mathbf{v} = \sigma \bar{\mathbf{u}}.$$

For the second part we mimic the steps used to obtain (52) and we also use (60). The last part follows from (56) with $z = \bar{r}_l$,

$$\overline{\mathbf{P}_u(r_l)} = \frac{(\mathbf{A}\mathbf{v})_l}{\sigma \bar{c}_l} = \frac{\bar{v}_l}{\bar{c}_l}. \quad \square$$

7. Approximation of power functions and separated representations

Let us discuss how to approximate the power functions $r^{-\alpha}$, $\alpha > 0$, with a linear combination of Gaussians,

$$\left| r^{-\alpha} - \sum_{m=1}^M w_m e^{-p_m r^2} \right| \leq r^{-\alpha} \varepsilon \tag{61}$$

for $r \in [\delta, 1]$. This approximation provides an example of an analytic construction of a separated representation as introduced in [9] and discussed in [10,23]. It also has ubiquitous applications and has already been used in the construction of a multiresolution separated representation for the Poisson kernel [8,15,16] and for the projector on the divergence free functions [8]. Setting $\alpha = 1$ in (61), we obtain the approximation of the Poisson kernel in \mathbb{R}^3 as a sum of separable functions,

$$\left| \frac{1}{\|x\|} - \sum_{m=1}^M w_m e^{-p_m \|x\|^2} \right| \leq \frac{\varepsilon}{\|x\|} \tag{62}$$

for $0 < \delta \leq \|x\| \leq 1$. It turns out that in some important applications, it is essential to obtain this approximation for small δ . By replacing r by $r^{1/2}$ in (61), the approximation becomes that in Section 4,

$$\left| r^{-\alpha/2} - \sum_{m=1}^M w_m e^{-p_m r} \right| \leq r^{-\alpha/2} \varepsilon \tag{63}$$

for $\delta^2 \leq r \leq 1$. Unfortunately, the algorithm of Section 4 is ill-suited to obtain (63) due to the large number of samples necessary to cover the range of interest. On the other hand, if we use the reduction procedure of Section 6, we only need an accurate, initial approximation to then minimize the number of nodes without experiencing the size constraints. Such initial approximation for (61) has been used in [8,15,16] and is based upon the discretization of the integral

$$r^{-\alpha} = \frac{2}{\Gamma(\alpha/2)} \int_{-\infty}^{\infty} e^{-r^2 e^{2s} + \alpha s} ds. \tag{64}$$

In this paper we analytically estimate the number of terms in (61) as a function of the accuracy and the range.

Since the integrand (64) has either exponential or super-exponential decay at the integration limits, for a given accuracy and range $0 < \delta \leq r \leq 1$, we select $a < 0$ and $b > 0$, the end points of the finite interval of integration, so that the discarded integrals are small and, at a and b both the integrand and a sufficient number of its derivatives are smaller than the desired accuracy. We also select K , the number of points in the quadrature, so that we can accurately discretize (64) by the trapezoidal rule, namely, by setting $p_k = e^{2s_k}$ and $w_k = \frac{2}{\Gamma(\frac{\alpha}{2})} e^{\alpha s_k} h$, where $s_k = a + kh$, $k = 0, \dots, K$ and $h = \frac{b-a}{K}$.

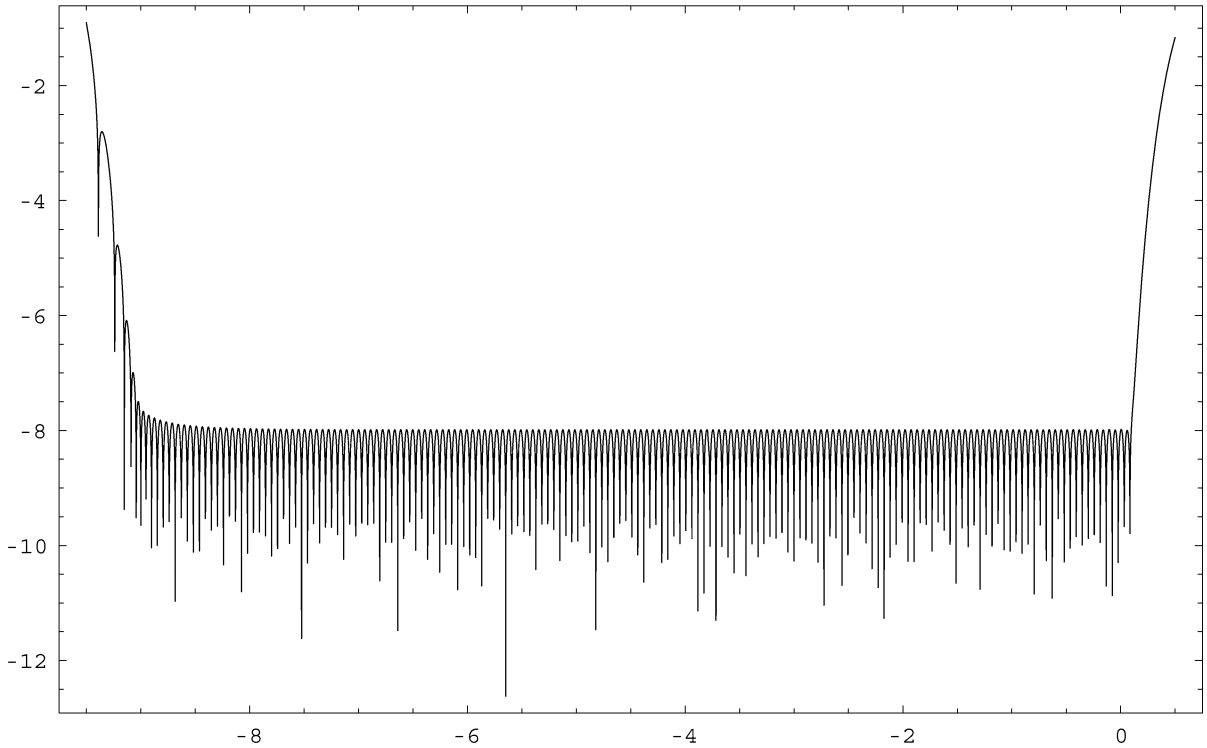


Fig. 9. Relative error (in logarithmic scale) of approximating the Poisson kernel in the range $10^{-9} \leq \|x\| \leq 1$ as a linear combination of 89 Gaussians.

Such explicit discretization is readily available but it is suboptimal. We then use the reduction procedure of Section 6 to minimize the number of terms and, if necessary, adjust the type of relative error in the estimate. As an example, in Fig. 9 we display the error in (62) after optimization. The number of terms is only $M = 89$ providing an uniform error in the whole range.

In order to estimate the number of terms in the approximation (61) of $r^{-\alpha}$ we demonstrate

Theorem 9. For any $\alpha > 0$, $0 < \delta \leq 1$, and $0 < \varepsilon \leq \min\{\frac{1}{2}, \frac{8}{\alpha}\}$, there exist positive numbers p_m and w_m such that

$$\left| r^{-\alpha} - \sum_{m=1}^M w_m e^{-p_m r^2} \right| \leq r^{-\alpha} \varepsilon \quad \text{for all } \delta \leq r \leq 1 \tag{65}$$

with

$$M = \log \varepsilon^{-1} [c_0 + c_1 \log \varepsilon^{-1} + c_2 \log \delta^{-1}], \tag{66}$$

where c_k are constants that only depend on α . For fixed power α and accuracy ε , we have $M = \mathcal{O}(\log \delta^{-1})$.

The proof (see Appendix A) is based on the fact that in (64) the integrand function

$$g_{\alpha,r}(s) = e^{-r^2 e^{2s} + \alpha s} \tag{67}$$

satisfy

$$D^n g_{\alpha,r}(s) = p_n^\alpha(-r^2 e^{2s}) g_{\alpha,r}(s),$$

where $p_n^\alpha(x)$ are polynomials of degree n .

Before ending this section, we would like to remark on another application of the reduction algorithm to the summation of slowly convergent series. These results will appear separately and here we only note that our approach yields an excellent rational approximation of functions like $r^{-\alpha}$, $\alpha > 0$, providing a numerical tool to obtain best order rational approximations as indicated by Newman [24] (see also [18, p. 169]).

8. Conclusions

We have introduced a new approach, and associated algorithms, for the approximation of functions and sequences by linear combination of exponentials with complex-valued exponents. Such approximations obtained for a finite but arbitrary accuracy may be viewed as representations of functions which are more efficient (significantly fewer terms) than the standard Fourier representations. These representations can be used for a variety of purposes. For example, if used to represent kernels of operators, these approximations yield fast algorithms for applying these operators to functions. For multi-dimensional operators, we have shown how the approximation of $r^{-\alpha}$, $\alpha > 0$ leads to separated representations of Green's functions (e.g., the Poisson kernel).

We note that we just began developing the theory of such approximations and there are still many questions to be answered. We have indicated some of these questions but, in this paper, instead of concentrating on the theoretical aspects we have chosen to emphasize examples and applications of these remarkable approximations.

Acknowledgments

We thank Dr. Brad Alpert (NIST) for pointing out connections with the steepest descent method and Dr. Martin Mohlenkamp (Ohio University) for many useful suggestions.

Appendix A

We show how to choose the parameters involved in the approximation of $r^{-\beta}$, $\beta > 0$ by linear combination of exponentials as well as estimate the number of terms. Theorem 9 follows by substituting $\beta \mapsto \frac{\alpha}{2}$, $r \mapsto r^2$, $\delta \mapsto \delta^2$ and choosing $N = \mathcal{O}(\log \varepsilon^{-1})$ in the next

Theorem A.1. *For any $\beta > 0$, $0 < \delta \leq 1$, and $0 < \varepsilon \leq \min\{\frac{1}{2}, \frac{4}{\beta}\}$, there exist positive numbers p_m and w_m such that*

$$\left| r^{-\beta} - \sum_{m=1}^M w_m e^{-p_m r} \right| \leq r^{-\beta} \varepsilon \quad \text{for all } \delta \leq r \leq 1 \quad (\text{A.1})$$

with

$$M \leq \frac{c_\beta(2N+1)}{\pi} [\beta^{-1} \log 4(\beta\varepsilon)^{-1} + \log 2q\delta^{-1} + \log(\log q(\delta\varepsilon)^{-1})], \quad (\text{A.2})$$

where

$$c_\beta = \begin{cases} 1, & 0 < \beta < 1, \\ \beta, & 1 \leq \beta, \end{cases} \quad (\text{A.3})$$

N is any positive integer chosen to satisfy

$$\frac{2N!}{(2N+1)^{2N}} \leq \frac{\varepsilon}{4}, \quad (\text{A.4})$$

and $q = 2N - 1 + \beta$.

For fixed power β and accuracy ε , we thus have $M = \mathcal{O}(\log \delta^{-1})$.

The approximation is based on the discretization of the integral representation of the function $r^{-\beta}$ for $\text{Re}(\beta) > 0$ and $r > 0$,

$$\Gamma(\beta)r^{-\beta} = \int_{-\infty}^{\infty} f_{\beta,r}(t) dt, \quad (\text{A.5})$$

where

$$f_{\beta,r}(t) = e^{-re^t + \beta t}.$$

The integral in (A.5) follows by substituting $x = re^t$ in the standard definition of the Gamma function,

$$\Gamma(\beta) = \int_0^{\infty} e^{-x} x^{\beta-1} dx.$$

Note that (64) is obtained substituting $\beta \mapsto \frac{\alpha}{2}$ and $r \mapsto r^2$ in (A.5).

Using the Euler–Maclaurin formula (see [6] or [14, pp. 469–475] for example), we approximate the integral of a smooth function $f(t)$ by the trapezoidal rule,

$$T_h^K = h \left(\sum_{k=1}^{K-1} f(a+kh) + \frac{f(a) + f(b)}{2} \right),$$

with the error given by

$$\begin{aligned} \int_a^b f(t) dt - T_h^K &= h^{2N+1} \int_0^K \frac{B_{2N}(t - [t])}{2N!} D^{2N} f(a+th) dt \\ &\quad - \sum_{n=1}^N \frac{b_{2n}}{2n!} h^{2n} (D^{2n-1} f(b) - D^{2n-1} f(a)), \end{aligned} \quad (\text{A.6})$$

where $h = \frac{b-a}{K}$ is the step size, $[t]$ is the integer part of the real number t , b_n are the Bernoulli numbers, and $B_n(t)$ the Bernoulli polynomials. For all $x \in [0, 1]$ and $n \geq 1$ we have the inequalities (see, e.g., [14, p. 474]),

$$\frac{|B_{2n}(x)|}{2n!} \leq \frac{|b_{2n}|}{2n!} = \frac{2}{(2\pi)^{2n}} \sum_{k \geq 1} k^{-2n} \leq 4(2\pi)^{-2n}.$$

We then estimate the error in (A.6) as

$$\left| \int_a^b f(t) dt - T_h^K \right| \leq 4 \left(\frac{h}{2\pi} \right)^{2N} \int_a^b |D^{2N} f(t)| dt + 4 \sum_{n=1}^N \left(\frac{h}{2\pi} \right)^{2n} (|D^{2n-1} f(b)| + |D^{2n-1} f(a)|). \tag{A.7}$$

Using (A.7) and (A.5), we obtain

$$|\Gamma(\beta)r^{-\beta} - T_h^K| \leq I_a + I_b + I + S_a + S_b, \tag{A.8}$$

where

$$I_a = \int_{-\infty}^a f_{\beta,r}(t) dt, \quad I_b = \int_b^{\infty} f_{\beta,r}(t) dt,$$

$$S_t = 4 \sum_{n=1}^N \left(\frac{h}{2\pi} \right)^{2n} |D^{2n-1} f_{\beta,r}(t)|, \quad I = 4 \left(\frac{h}{2\pi} \right)^{2N} \int_{-\infty}^{\infty} |D^{2N} f_{\beta,r}(t)| dt.$$

We will derive conditions on the parameters a, b, K , and N so that the first four terms in the estimate (A.8) are less than $\frac{\varepsilon}{6}$ and the last term is less than $\Gamma(\beta)r^{-\beta} \frac{\varepsilon}{6}$ for all $r, \delta \leq r \leq 1$. Since for $\beta > 0$ and $0 < r \leq 1, r^{-\beta} \Gamma(\beta) \geq \Gamma(\beta) \geq 0.886 \dots > 4/5$, we obtain

$$|\Gamma(\beta)r^{-\beta} - T_h^K| \leq 4 \frac{\varepsilon}{6} + \Gamma(\beta)r^{-\beta} \frac{\varepsilon}{6} < \Gamma(\beta)r^{-\beta} \varepsilon,$$

and (A.1). To obtain these estimates, we use some auxiliary results collected in

Lemma A.2. *The derivatives of the function $f_{\beta,r}$ are*

$$D^n f_{\beta,r}(t) = F_n^\beta(-re^t) f_{\beta,r}(t), \tag{A.9}$$

where $F_n^\beta(x)$ are polynomials of degree n , satisfying the recurrence

$$F_{n+1}^\beta(x) = x F_n^{\beta+1}(x) + \beta F_n^\beta(x), \tag{A.10}$$

with $F_0^\beta(x) = 1$. These polynomials can be written as

$$F_n^\beta(x) = \sum_{k=0}^n A_k^n(\beta) x^k, \tag{A.11}$$

with nonnegative coefficients

$$A_k^n(\beta) = \sum_{j=k}^n \binom{n}{j} S_k^j \beta^{n-j}, \tag{A.12}$$

where S_k^j are the Stirling numbers of the second kind, $S_0^j = \delta_{j0}$ and $S_k^j = 0$ if $k > j$. These combinatorial numbers satisfy [14, Eq. 6.15 and 7.47],

$$\sum_{j=k}^n \binom{n}{j} S_k^j = S_{k+1}^{n+1}, \tag{A.13}$$

$$\sum_{n=k}^{\infty} S_k^n z^k = \frac{1}{\prod_{l=1}^k (z^{-1} - l)} \quad \text{for } |z| < \frac{1}{k}. \tag{A.14}$$

Properties of the polynomials F_n^β can be easily derived from the relationships

$$F_n^\beta(x) = a_n^{(\beta)}(-x) = \sum_{j=0}^n \binom{n}{j} \beta^{n-j} \phi_j(x),$$

where $a_n^{(\beta)}$ are the actuarial polynomials [26, pp. 123–125] and ϕ_j are the exponential polynomials [26, pp. 63–69]. Let us now establish conditions, to bound each of the five terms in (A.8).

A.1. Condition for $I_a < \varepsilon$

We have $\int_{-\infty}^a e^{-re^t} e^{\beta t} dt \leq \int_{-\infty}^a e^{\beta t} dt = \frac{e^{\beta a}}{\beta} < \varepsilon$, if the left end of the interval of integration satisfies

$$a < \frac{\ln(\varepsilon\beta)}{\beta}. \tag{A.15}$$

A.2. Condition for $I_b < \varepsilon$

If we denote $L = [\beta]$, then $I_b = \int_b^\infty e^{-re^t} e^{\beta t} dt \leq \int_b^\infty e^{-\delta e^t} e^{(L+1)t} dt = \delta^{-L-1} \int_{\delta e^b}^\infty e^{-s} s^L ds$. Integrating by parts L times, we have

$$\delta^{-L-1} \int_{\delta e^b}^\infty e^{-s} s^L ds = \delta^{-L-1} E_L(\delta e^b) e^{-\delta e^b},$$

where $E_L(x) = \sum_{l=0}^L \frac{x^l}{l!}$. Note that $E_L(x) \leq ex^L$ for $x \geq 1$. Assuming

$$\delta e^b \geq e, \tag{A.16}$$

we obtain $I_b < \varepsilon$ provided the right end of the interval of integration satisfies

$$e^{([\beta]+1)b} e^{-\delta e^b} < \varepsilon. \tag{A.17}$$

A.3. Estimates for $S_t < \varepsilon$, for $t = a$ and $t = b$

Using (A.9) and (A.11), for $r \leq 1$, we have

$$S_t \leq 4f_{\beta,r}(t) \sum_{n=1}^N \left(\frac{h}{2\pi}\right)^{2n} \sum_{k=0}^{2n-1} A_k^{2n-1}(\beta) r^k e^{tk} \leq 4e^{\beta t - re^t} \sum_{n=1}^N \left(\frac{h}{2\pi}\right)^{2n} \sum_{k=0}^{2n-1} A_k^{2n-1}(\beta) e^{tk}. \tag{A.18}$$

Denoting

$$d_h = \sum_{n=1}^N \left(\frac{h}{2\pi}\right)^{2n} \sum_{k=0}^{2n-1} A_k^{2n-1}(\beta),$$

let us show that $d_h \leq 1/c_\beta$ if

$$c = \frac{hc_\beta}{2\pi} \leq \frac{1}{2N+1}. \tag{A.19}$$

Using (A.12) and (A.13), we obtain

$$\begin{aligned} d_h &\leq \sum_{n=1}^N \left(\frac{h}{2\pi}\right)^{2n} c_\beta^{2n-1} \sum_{k=0}^{2n-1} \sum_{j=k}^{2n-1} \binom{2n-1}{j} S_k^j = \frac{1}{c_\beta} \sum_{n=1}^N c^{2n} \sum_{k=1}^{2n} S_k^{2n} \\ &= \frac{1}{c_\beta} \sum_{k=1}^{2N} \sum_{n=1}^N S_k^{2n} c^{2n} \leq \frac{1}{c_\beta} \sum_{k=1}^{2N} \sum_{n=k}^{\infty} S_k^n c^n. \end{aligned}$$

Since we have assumed (A.19), with (A.14) for all $1 \leq k \leq 2N$, we estimate

$$\sum_{k=1}^{2N} \sum_{n=k}^{\infty} S_k^n c^n = \sum_{k=1}^{2N} \frac{1}{\prod_{l=1}^k (c^{-1} - l)} \leq \sum_{k=1}^{2N} \frac{1}{\prod_{l=1}^k (2N+1-l)} \leq 1,$$

where the last inequality follows by induction on N .

Under the condition (A.19), we consider two cases in (A.18). If $t = a < 0$,

$$S_a \leq 4e^{\beta a} d_h \leq \frac{4}{c_\beta} e^{\beta a}$$

and to obtain $S_a < \varepsilon$, we need

$$a < \frac{1}{\beta} \ln\left(\frac{\varepsilon c_\beta}{4}\right).$$

Since $\beta \leq c_\beta$, we obtain both the last inequality and (A.15) by requiring

$$a < \frac{1}{\beta} \ln\left(\frac{\varepsilon \beta}{4}\right), \tag{A.20}$$

which, due to the assumptions on ε , ensures that the left end of the interval of integration is negative.

If $t > 0$ and denoting $q = 2N - 1 + \beta \geq [\beta] + 1$, we have

$$S_t \leq 4e^{\beta t - r e^t} d_h \leq \frac{4}{c_\beta} e^{\beta t} e^{-\delta e^t} e^{(2N-1)t} = \frac{4}{c_\beta} e^{qt} e^{-\delta e^t} \leq 4e^{qt} e^{-\delta e^t},$$

and thus we obtain both, inequality (A.17) and $S_b < \varepsilon$ provided that

$$\ln\left(2q\delta^{-1} \ln\left(q\delta^{-1} \left(\frac{\varepsilon}{4}\right)^{-\frac{1}{q}}\right)\right) < b,$$

a condition that follows from Lemma A.3 below. Since $\varepsilon \leq \frac{1}{2}$, assumption (A.4) implies that $N \geq 2$ and, therefore, $(\frac{\varepsilon}{4})^{-\frac{1}{q}} \leq \varepsilon^{-1}$. Therefore, we set the following condition for the right end of the interval of integration,

$$\ln(2q\delta^{-1} \ln(q(\delta\varepsilon)^{-1})) < b, \tag{A.21}$$

which also implies (A.16).

Lemma A.3. *Let $p, \delta,$ and ε be positive numbers such that $p\delta^{-1}\varepsilon^{-\frac{1}{p}} \geq e^{\frac{1}{2}}$ and define $t_0 = \ln 2p\delta^{-1} \times \ln(p\delta^{-1}\varepsilon^{-\frac{1}{p}})$. Then the inequality*

$$e^{pt} e^{-\delta e^t} < \varepsilon \tag{A.22}$$

holds for all $t \geq t_0$.

Taking the logarithm in both sides of (A.22) we get $t - \frac{\delta e^t}{p} < \frac{\ln \varepsilon}{p}$, and introducing the new variable $x = \frac{\delta e^t}{p} \geq 1$, we obtain

$$\ln(p\delta^{-1}x) - x < \frac{\ln \varepsilon}{p} \tag{A.23}$$

or

$$c = \ln p\delta^{-1}\varepsilon^{-\frac{1}{p}} < x - \ln x.$$

Since $1 - x \leq -\ln x$ for positive x , we have

$$c < 2c - \ln 2 + (1 - c) \leq 2c - \ln(2c),$$

and, thus, (A.23) holds for $x \geq 2c$ since $x - \ln x$ is increasing for $x \geq 1$.

A.4. Condition for I and selection of the step size h

Let us show by induction on $n \geq 0$, that for all $\beta > 0$

$$\int_{-\infty}^{\infty} |D^n f_{\beta,r}(t)| dt \leq \int_{-\infty}^{\infty} |F_n^\beta(-re^t)| f_{\beta,r}(t) dt \leq \Gamma(\beta + n)r^{-\beta}2^n. \tag{A.24}$$

The case $n = 0$ follows from (A.5) and, using the recurrence (A.10) and the induction assumption, we have

$$\begin{aligned} \int |F_{n+1}^\beta(-re^t)| f_{\beta,r}(t) dt &\leq r \int |F_n^{\beta+1}(-re^t)| f_{\beta+1,r}(t) dt + \beta \int |F_n^\beta(-re^t)| f_{\beta,r}(t) dt \\ &\leq r\Gamma(\beta + 1 + n)r^{-\beta-1}2^n + \beta\Gamma(\beta + n)r^{-\beta}2^n \\ &\leq \Gamma(\beta + n + 1)r^{-\beta}2^n + (\beta + n)\Gamma(\beta + n)r^{-\beta}2^n. \end{aligned}$$

Observing that

$$\Gamma(\beta + n) \leq n!\Gamma(\beta)c_\beta^n, \tag{A.25}$$

where c_β is defined in (A.3) and denoting $L = 2N$, we estimate I as

$$I \leq 4 \left(\frac{h}{2\pi} \right)^L \Gamma(\beta + L) r^{-\beta} 2^L \leq 4 \left(\frac{hc_\beta}{\pi} \right)^L L! \Gamma(\beta) r^{-\beta} \leq \varepsilon \Gamma(\beta) r^{-\beta},$$

provided

$$\frac{hc_\beta}{2\pi} \leq \frac{1}{2} \left(\frac{\varepsilon}{L!4} \right)^{\frac{1}{L}}.$$

Using (A.4), we satisfy both the last inequality and (A.19) if the step size satisfies

$$h \leq \frac{1}{c_\beta} \frac{\pi}{2N + 1}. \quad (\text{A.26})$$

Finally, the sampling rate $K = \frac{b-a}{h}$ and, therefore, the number of terms in (A.1) can be chosen as to verify (A.2) if we collect the estimates (A.20), (A.21), and (A.26).

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