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NUMERICAL TRANSFORM INVERSION USING GAUSSIAN QUADRATURE

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Numerical inversion of Laplace transforms is a powerful tool in computational probability. It greatly enhances the applicability of stochastic models in many fields. In this article we present a simple Laplace transform inversion algorithm that can compute the desired function values for a much larger class of Laplace transforms than the ones that can be inverted with the known methods in the literature. The algorithm can invert Laplace transforms of functions with discontinuities and singularities, even if we do not know the location of these discontinuities and singularities a priori. The algorithm only needs numerical values of the Laplace transform, is extremely fast, and the results are of almost machine precision. We also present a two-dimensional variant of the Laplace transform inversion algorithm. We illustrate the accuracy and robustness of the algorithms with various numerical examples.

1. INTRODUCTION

The emphasis on computational probability increases the value of stochastic models in queuing, reliability, and inventory problems. It is becoming standard for modeling and analysis to include algorithms for computing probability distributions of interest. Several tools have been developed for this purpose. A very powerful tool is numerical Laplace inversion. Probability distributions can often be characterized

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in terms of Laplace transforms. Many results in queuing and reliability among others are given in the form of transforms and become amenable for practical computations once fast and accurate methods for numerical Laplace inversion are available. Numerical Laplace inversion is much easier to use than it is often made to seem. This article presents a new and effective algorithm for numerical Laplace inversion. The new algorithm outperforms existing methods, particularly when the function to be inverted involves discontinuities or singularities, as is often the case in applications.

The algorithm can compute the desired function values $f(k\Delta)$, $k = 0,1,\ldots,M-1$ for a much larger class of Laplace transforms than the ones that can be inverted with the known methods in the literature. It can invert Laplace transforms of functions with discontinuities and singularities, even if we do not know the location of these discontinuities and singularities a priori, and also locally nonsmooth and unbounded functions. It only needs numerical values of the Laplace transform, the computations cost $M\log(M)$ time, and the results are near machine precision. This is especially useful in applications in computational finance, where one needs to compute a large number of function values by transform inversion (cf. Carr and Madan [8]). With the existing Laplace transform inversion methods, this is very expensive. With the new method, one can compute the function values $f(k\Delta)$, $k = 0,1,\ldots,M-1$, at once in $M\log(M)$ time.

There are many known numerical Laplace inversion algorithms. Four widely used methods are (1) the Fourier series method, which is based on the Poisson summation formula (cf. Dubner and Abate [13], Abate and Whitt [4,5], Choudhury, Lucantoni, and Whitt [9], O'Cinneide [17], and Sakurai [21]), (2) the Gaver-Stehfest algorithm, which is based on combinations of Gaver functionals (cf. Gaver [14] and Stehfest [22]), (3) the Weeks method, which is based on bilinear transformations and Laguerre expansions (cf. Weeks [27] and Abate, Choudhury, and Whitt [1,2]), and (4) the Talbot method, which is based on deforming the contour in the Bromwich inversion integral (cf. Talbot [25] and Murli and Rizzardi [16]).

The new algorithm is based on the well-known Poisson summation formula and can therefore be seen as a so-called Fourier series method, developed in the 1960s by Dubner and Abate [13]. The Poisson summation formula relates an infinite sum of Laplace transform values to the z-transform (Fourier series) of the function values $f(k\Delta)$, $k = 0,1,\ldots$. Unfortunately, the infinite sum of Laplace transform values, in general, converges very slowly. In their seminal article, Abate and Whitt [4] used an acceleration technique called Euler summation to accelerate the convergence rate of the infinite sum of Laplace transform values. Recently, Sakurai [21] extended the Euler summation to be effective for a wider class of functions. A disadvantage of all the variants of the Fourier series methods is that unless one has specified information about the location of singularities, the accelerating techniques are not very effective and the convergence is slow.

We present a Gaussian quadrature rule for the infinite sum of Laplace transform values. The Gaussian quadrature rule approximates accurately the infinite sum with a finite sum. Then we compute the function values $f(k\Delta)$, $k = 0,1,\ldots,M-1$,

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efficiently with the well-known fast Fourier transform (FFT) algorithm (cf. Cooley and Tukey [11]). For smooth functions, the results are near machine precision. With a simple modification, we can handle known discontinuities in the points $k\Delta$, $k = 0,1,\ldots$, such that the running time of the algorithm is still insensitive to the number of discontinuities and we get results near machine precision. We also extend the Gaussian quadrature formula for the multidimensional Laplace transform and present a multidimensional Laplace transform inversion algorithm. With this algorithm, we can compute the function values $f(k_1\Delta_1,\ldots,k_j\Delta_j)$, $k_j = 0,1,\ldots,M-1$, at once in $M^j\log(M^j)$ time and the results are again of machine precision. We develop a modification that gives results near machine precision for functions with singularities and discontinuities on arbitrary locations. We also develop a modification that is effective for almost all kinds of discontinuity, singularity, and local non-smoothness. With this modification, we can obtain results near machine precision in continuity points for almost all functions, even if we do not know the location of these discontinuities and singularities a priori.

The accurateness and robustness of the algorithms is illustrated by examining all of the Laplace transforms that are used in the overview article of Davies and Martin (cf. [12]). We also demonstrate the effectiveness of the algorithm with an application in queuing theory by computing the waiting time distribution for a $M/D/1$ queue.

2. OUTLINE OF THE METHOD

Let f be a complex-valued Lebesgue integrable function f, with $e^{-\alpha t}f(t) \in L^1[0,\infty)$, for all $\alpha > c$. The Laplace transform of f is defined by the integral

$$\hat{f}(s) := \int_0^\infty e^{-st}f(t)\,dt, \qquad \mathrm{Re}(s) > c. \tag{2.1}$$

The Poisson summation formula relates an infinite sum of Laplace transform values to the z-transform (damped Fourier series) of the function values $f(k\Delta)$, $k = 0,1,\ldots.$

THEOREM 2.1 (PSF): *Suppose that $f \in L^1[0,\infty)$ and f is of bounded variation. Then for all $v \in [0,1)$,*

$$\sum_{k=-\infty}^{\infty} \hat{f}(a + 2\pi i(k+v)) = \sum_{k=0}^{\infty} e^{-ak}e^{-i2\pi kv}f(k); \tag{2.2}$$

here, $f(t)$ has to be understood as $(f(t^+)+f(t^-))/2$, the so-called damping factor a is a given real number, and i denotes the imaginary number $\sqrt{-1}$.

A proof of this classical result can, for instance, be found in Abate and Whitt [4] or Mallat [15]. The right-hand side of (2.2) is the (damped) Fourier series of the function values $\{f(k); k = 0,1,\ldots\}$. In this article we present a Gaussian quadrature

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rule for the left-hand side of (2.2); that is, we approximate this infinite sum with a finite sum,

$$\sum_{k=1}^{n} \beta_k \hat{f}(a + i\lambda_k + 2\pi i v),$$

with $\{\beta_k\}$ given positive numbers and the $\{\lambda_k\}$ given real numbers. In Appendix A the reader can find these numbers for various values of n. We can compute the function values $\{f(k); k = 0,1,\ldots,M-1\}$ by

$$\frac{e^{ak}}{M_2} \sum_{j=0}^{M_2-1} \cos\left(\frac{2\pi jk}{M_2}\right) \sum_{l=1}^{n} \beta_l \hat{f}\left(a + i\lambda_l + \frac{2\pi ij}{M_2}\right); \tag{2.3}$$

here, M_2 is a given power of 2. With the well-known FFT algorithm (cf. Cooley and Tukey [11]) we can compute these sums in $M_2 \log(M_2)$ time. We can compute the function values $f(k\Delta)$, $k = 0,1,\ldots,$ by applying (2.3) to the scaled Laplace transform

$$\hat{f}_\Delta(s) = \frac{1}{\Delta} \hat{f}\left(\frac{s}{\Delta}\right),$$

which is the Laplace transform of the function $f_\Delta(t) = f(\Delta t)$.

3. THE GAUSSIAN QUADRATURE RULE

We associate with the left-hand side of (2.2) an inner product, say $\langle \cdot,\cdot \rangle_{Q_v}$.

Definition 3.1: *Let the inner product* $\langle \cdot,\cdot \rangle_{Q_v}$ *be given by*

$$\langle f, g \rangle_{Q_v} = \sum_k \frac{1}{|2\pi(k+v)|^2} f\left(\frac{1}{2\pi i(k+v)}\right) g^*\left(\frac{1}{2\pi i(k+v)}\right).$$

Having $\mathbf{1}(s) = 1$ and $\Psi\hat{f}(s) = s^{-1}\hat{f}(s^{-1})$, we can write the left-hand side of (2.2) as $\langle \Psi\hat{f}, \Psi\mathbf{1} \rangle_{Q_v}$. The idea is to approximate this inner product with a Gaussian quadrature rule. As usual, we associate with the inner product $\langle \cdot,\cdot \rangle_{Q_v}$ the norm $\|\cdot\|_{Q_v}$, which induced the sequence space $L^2(Q_v)$. We say that a function f belongs to $L^2(Q_v)$ iff the sequence $\{f(1/2\pi i(k+v))\}$ belongs to $L^2(Q_v)$. Let the polynomials $\{q_n^v; n \in N_0\}$ be given by

$$q_n^v(s) := p_n(s) - (-1)^n e^{-i2\pi v} p_n(-s),$$

where

$$p_n(s) = \sqrt{2n+1} \sum_{k=0}^{n} \frac{(k+n)!}{(n-k)!} \frac{(-s)^k}{k!}.$$

The following result holds.

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THEOREM 3.2: *The set* $\{q_j^v; j = 0,1,\ldots\}$ *is a complete orthogonal set of polynomials in* $L^2(Q_v)$.

The proof is given in Appendix E.

We can now easily obtain the desired Gaussian quadrature rule (cf. Definition C.1 in Appendix C). We denote this quadrature rule with $\langle \cdot,\cdot \rangle_{Q_v^n}$.

DEFINITION 3.3: *The inner product* $\langle \cdot,\cdot \rangle_{Q_v^n}$ *is given by*

$$\langle f,g \rangle_{Q_v^n} = \sum_{k=1}^{n} \alpha_k^v \hat{f}(\mu_k^v)\hat{g}^*(\mu_k^v).$$

The $\{\mu_k^v\}$ *are the zeros of the polynomial* q_n^v. *The so-called Christophel numbers* $\{\alpha_k^v\}$ *are positive numbers given by*

$$\alpha_k^v = \frac{1}{\sum_{j=1}^{n} |q_j^v(\mu_k^v)|^2}. \tag{3.1}$$

It is well known (cf. Szegő [24]) that the roots of orthogonal polynomials are all distinct and lie on the support of the inner product; thus, the roots $\{\mu_k^v\}$ are all distinct and lie on the imaginary axis. Having $\mathbf{1}(s) = 1$ and $\Psi\hat{f}(s) = s^{-1}\hat{f}(s^{-1})$, we approximate $\langle \Psi\hat{f}, \Psi\mathbf{1} \rangle_{Q_v}$ with our Gaussian quadrature rule and obtain the quadrature formula

$$\sum_{k=1}^{n} \frac{\alpha_k^v}{|\mu_k^v|^2} \hat{f}\left(\frac{1}{\mu_k^v}\right) \approx \sum_{k=-\infty}^{\infty} \hat{f}(2\pi i(k+v)) = \sum_{k=0}^{\infty} \exp(-2\pi ikv) f(k),$$

where the last identity follows from the PSF formula (2.2). In Appendix F we explain how we can compute the numbers $\{\mu_k^v\}$ and $\{\alpha_k^v\}$ efficiently. Considering that only the real part yields the quadrature formula

$$\sum_{k=1}^{n} \frac{\alpha_k^v}{|\mu_k^v|^2} \mathrm{Re}\left(\hat{f}\left(\frac{1}{\mu_k^v}\right)\right) \approx \sum_{k=0}^{\infty} \cos(2\pi kv) f(k), \tag{3.2}$$

we used here that the α_k^v are real. Similarly to the Abate and Whitt algorithm (cf. [4]), we use a damping factor for functions with support contained in $[0,\infty)$; that is, we take the Laplace transform $\hat{f}(a+s)$, which is the Laplace transform of $e^{-at}f(t)$. This yields the quadrature rule

$$F_a(v) \approx \sum_{k=0}^{\infty} e^{-ak} \cos(2\pi kv) f(k), \tag{3.3}$$

where

$$F_a(v) = \sum_{k=1}^{n} \frac{\alpha_k^v}{|\mu_k^v|^2} \mathrm{Re}\left(\hat{f}\left(a + \frac{1}{\mu_k^v}\right)\right).$$

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It remains to compute the function values $f(k)$, $k = 0, 1, \ldots, M-1$. We can realize this by the discrete Fourier series inversion formula

$$f(k) \approx \frac{e^{ak}}{M_2} \sum_{j=0}^{M_2-1} \cos\left(\frac{2\pi\left(j+\frac{1}{2}\right)k}{M_2} \right) F_a\left(\frac{j+\frac{1}{2}}{M_2} \right), \tag{3.4}$$

with M_2 a given power of 2. With the well-known FFT algorithm (cf. Cooley and Tukey [11]), we can compute the sums (3.4) in $M_2 \log(M_2)$ time. In Appendix H we discuss the details of this approach.

Remark 3.4: The quadrature rule is also valid for a function f with support $(-\infty, \infty)$. Formula (3.3) then reads as

$$F_a(v) \approx \sum_{k=-\infty}^{\infty} \cos(2\pi k v) e^{-ak} f(k\Delta).$$

Remark 3.5: For smooth functions on $(-\infty, \infty)$ or $[0, \infty)$, the quadrature formula is extremely accurate. In Appendix G and, in particular, Theorem G.3 we prove that for smooth functions, the approximation error of (3.3) is approximately

$$\frac{1}{2}(-1)^n \frac{(n-1)!\,n!}{(2n-1)!} \sum_{j=1}^{\infty} j e^{-i2\pi j v} \frac{f^{(2n+1)}(j-1+\alpha)}{(2n+1)!}, \tag{3.5}$$

with α some number in $(0,2)$. This implies that if we compute the function values $f(k\Delta)$, $k = 0, 1, \ldots$, by inverting the Laplace transform

$$\hat{f}_\Delta(s) = \frac{1}{\Delta} \hat{f}\left(\frac{s}{\Delta} \right),$$

with (3.4), the approximation error is of the order $O(\Delta^{2n+1})$. Formula (3.5) shows also that if

$$\frac{f^{(2n+1)}(j-1+\alpha)}{(2n+1)!}$$

is bounded, then the quadrature formula converges faster than any power of n.

Remark 3.6: The convergence of the quadrature rule is insensitive for discontinuity in $t = 0$ (cf. Remark G.4 in Appendix G).

Remark 3.7: Gaussian quadrature is a standard method for the numerical evaluation of integrals (cf. Stoer and Bulirsch [23]). Piessens (cf. [18,19]) tried to apply Gaussian quadrature directly on the Bromwich inversion integral. He reports in [19] for the first Laplace transform of Table 1 (cf. Section 4.2) an average approximation error of 1.0e-4 for a 17-point quadrature rule (for the values

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TABLE 1. Results for Analytical Test Functions

No.	Function	Laplace Transform
1	$J_0(x)$	$(s^2+1)^{-1/2}$
2	$\exp(-x/2)$	$(s+\frac{1}{2})^{-1}$
3	$\exp(-0.2x)\sin(x)$	$((s+0.2)^2+1)^{-1}$
4	1	s^{-1}
5	x	s^{-2}
6	$x\exp(-x)$	$(s+1)^{-2}$
7	$\sin(x)$	$(s^2+1)^{-1}$
8	$x\cos(x)$	$(s^2-1)(s^2+1)^{-2}$

No.	$\Delta = 1/16$	$\Delta = 1$	$\Delta = 10$
1	1e-15	1e-15	5e-13
2	1e-15	1e-15	3e-16
3	2e-16	1e-15	3e-12
4	1e-15	1e-15	1e-15
5	3e-15	5e-15	6e-15
6	2e-16	3e-16	2e-16
7	1e-15	1e-15	5e-12
8	4e-16	6e-15	2e-12

Note: The mean absolute error $\sum_{k=0}^{M-1}|e(k\Delta)|/(1+e(k\Delta))$ is presented for the inversion of eight analytical functions in the points $\{0, 1/16, \ldots, 31/16\}$, $\{0, 1, \ldots, 31\}$, and $\{0, 10, \ldots, 310\}$. From this table, we can conclude that for analytical functions, the results are almost of machine accuracy.

$t = 0, 1, \ldots, 12$). Our method gives an average approximation error of 1.0e-15 (cf. Table 1).

4. A SIMPLE LAPLACE TRANSFORM INVERSION ALGORITHM

In this section we explain how we can approximate the quadrature rule (3.2) with a simpler quadrature rule. In addition to this approximation being easier to implement, it is also numerically more stable. Therefore, we strongly recommend using this quadrature rule.

4.1. The Algorithm

We start by writing the PSF (cf. (2.2)) as

$$\sum_{k=-\infty}^{\infty} \hat{f}_{\rho_v^a}(i(2k+1)\pi) = \sum_{k=0}^{\infty} e^{-ak} e^{-i2\pi k v} f(k), \tag{4.1}$$

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with

$$\hat{f}_{\rho_v^a}(s) = \hat{f}(\rho_v^a + s), \qquad \rho_v^a = a + 2\pi i\left(v - \frac{1}{2}\right). \tag{4.2}$$

Applying the quadrature rule on the left-hand side of (4.1) yields the approximation

$$\sum_{k=1}^{n} \beta_k \hat{f}(i\lambda_k + a + 2\pi i v) \approx \sum_{k=0}^{\infty} e^{-i2\pi k v} e^{-ak} f(k), \tag{4.3}$$

with

$$\lambda_k = \frac{1}{i\mu_k^{0.5}} - \pi \quad \text{and} \quad \beta_k = \frac{\alpha_k^{0.5}}{|\mu_k^{0.5}|^2}. \tag{4.4}$$

Considering only the real part yields the formula

$$F_a(v) \approx \sum_{k=0}^{\infty} \cos(2\pi k v) e^{-ak} f(k), \tag{4.5}$$

with

$$F_a(v) = \sum_{k=1}^{n} \beta_k \operatorname{Re}(\hat{f}(a + i\lambda_k + 2\pi i v)). \tag{4.6}$$

We make F_a periodic by defining $F_a(0)$ and $F_a(1)$ equal to

$$\sum_{k=1}^{n} \beta_k \frac{1}{2} \operatorname{Re}(\hat{f}(a + i\lambda_k) + \hat{f}(a + i\lambda_k + 2\pi i)).$$

It remains to compute the function values $f(k)$, $k = 0, 1, \ldots, M - 1$. We can realize this by the discrete Fourier series inversion formula

$$f(k) \approx \frac{e^{ak}}{M_2} \sum_{j=0}^{M_2 - 1} \cos\left(\frac{2\pi jk}{M_2}\right) F_a\left(\frac{j}{M_2}\right), \tag{4.7}$$

with M_2 a given power of 2.

Finally, we show how to simplify (4.7). Since the coefficients of the polynomials $q_k^{0.5}$, $k = 1, 2, \ldots$, are real, we can order the roots $\{\mu_k^v\}$ such that the $\mu_k^{0.5}$ and $\mu_{n-k}^{0.5}$ are pairs of conjugate numbers. It follows from (3.1) that the Christophel numbers $\alpha_k^{0.5}$ and $\alpha_{n-k}^{0.5}$ are equal. Using this symmetry, (4.4), and the symmetry $\cos(2\pi v) = \cos(2\pi(1 - v))$ yields (for n is even) that (4.7) can be simplified to

$$f(k) \approx \frac{e^{ak}}{M_2} \sum_{j=0}^{M_2 - 1} \cos\left(\frac{2\pi jk}{M_2}\right) \tilde{F}_a\left(\frac{j}{M_2}\right), \tag{4.8}$$

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where

$$\tilde{F}_a(v) = \begin{cases} 2\sum_{k=1}^{n/2} \beta_k \operatorname{Re}(\hat{f}(a + i\lambda_k + i2\pi v)), & 0 < v < 1 \\ \sum_{k=1}^{n/2} \beta_k \operatorname{Re}(\hat{f}(a + i\lambda_k) + \hat{f}(a + i\lambda_k + i2\pi)), & v = 0. \end{cases}$$

In Appendix A the reader can find these numbers for various values of n. With the well-known FFT algorithm (cf. Cooley and Tukey [11]), we can compute the sums (4.8) in $M_2 \log(M_2)$ time. In Appendix H we discuss the details of the discrete Fourier inversion formula (4.8). We can now present our Laplace inversion algorithm.

Algorithm

Input: $\hat{f}$, Δ, and M, with M a power of 2
Output: $f(\ell\Delta)$, $\ell = 0,1,\ldots,M-1$
Parameters: $M_2 = 8M$, $a = 44/M_2$, and $n = 16$

Step 1. For $k = 0,1,\ldots,M_2$ and $j = 1,2,\ldots,n/2$, compute the numbers

$$\hat{f}_{jk} = \operatorname{Re}\left[\hat{f}\left(\frac{a + i\lambda_j + \frac{2i\pi k}{M_2}}{\Delta}\right)\right], \qquad \hat{f}_k = \frac{2}{\Delta}\sum_{j=1}^{n/2} \beta_j \hat{f}_{jk},$$

and $\hat{f}_0 = \frac{1}{\Delta}\sum_{j=1}^{n/2} \beta_j (\hat{f}_{j0} + \hat{f}_{jM_2}).$

Step 2. For $\ell = 0,1,\ldots,M_2 - 1$, compute the numbers

$$f_\ell = \frac{1}{M_2}\sum_{k=0}^{M_2-1} \hat{f}_k \cos\left(\frac{2\pi\ell k}{M_2}\right)$$

with the backwards FFT algorithm.

Step 3. Set $f(\ell\Delta) = e^{a\ell} f_\ell$ for $\ell = 0,1,\ldots,M-1$.

In Appendix H we discuss the details of Steps 2 and 3 of the algorithm.

Remark 4.1: We can compute the function values $f(k\Delta)$, $k = 0,1,\ldots,$ by applying the quadrature rule to the scaled Laplace transform

$$\hat{f}_\Delta(s) = \frac{1}{\Delta}\hat{f}\left(\frac{s}{\Delta}\right).$$

Remark 4.2: Extensive numerical experiments show that $n = 16$ gives, for all smooth functions, results attaining the machine precision. For double precision, we choose $a = 44/M_2$ and $M_2 = 8M$. For $n = 16$, we need 8 Laplace transform values for the quadrature rule and we use an oversampling factor of $M_2/M = 8$; thus, on average,

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we need 64 Laplace transform values for the computation of 1 function value. The method can be efficiently implemented with modern numerical libraries with FFT routines and matrix/vector multiplication routines (BLAS). If we are satisfied with less precision, then we can reduce the oversampling factor and/or the number of quadrature points. For other machine precisions, it is recommend to choose a somewhat larger than $-\log(\epsilon)/M_2$, with ϵ the machine precision.

Remark 4.3: The choice of the parameter M_2 is a trade-off between the running time and the accuracy of the algorithm. The actual running time is $M_2 \log(M_2)$; hence, from this perspective, we want to choose M_2 as small as possible. However, in Step 3 of the algorithm we multiply the results with a factor $\exp(a\ell) = \exp(44\ell/M_2)$; to obtain a numerically stable algorithm, we want to choose M_2 as large as possible. We recommend choosing $M_2 = 8M$.

Remark 4.4: Since the Gaussian quadrature rule is exact on the space of polynomials of degree $2n - 1$ or less, we obtain that

$$\sum_{k=1}^{n} \alpha_k^v = \langle \mathbf{1}, \mathbf{1} \rangle_{Q_v^n} = \langle \mathbf{1}, \mathbf{1} \rangle_{Q_v} = \frac{\langle q_0^v, q_0^v \rangle}{1 - \cos(2\pi v)} = \frac{1}{1 - \cos(2\pi v)}.$$

This is clearly minimal for $v = 0.5$. This shows that (4.6) is numerically more stable than the original Gaussian quadrature formula.

Remark 4.5: If n is odd, then one of the $\{\mu_k^{0.5}; k = 1, 2, \ldots, n\}$ is equal to zero. The evaluation of (3.2) can be a problem in this case. To avoid this, we take n even.

Remark 4.6: The Gaussian quadrature formula (3.3) is extremely accurate for smooth inverse functions (cf. Appendix G and Remark 3.5). Since the smoothness of the inverse function f implies that the function

$$e^{-s_v^a t} f(t) \quad \text{with } s_v^a = a + 2\pi v i \tag{4.9}$$

is a smooth function too, we can expect that the modified quadrature formula is extremely accurate for smooth functions. All of the numerical examples support this statement (cf. Section 4.2). In fact, many numerical experiments show that the modified formula performs even better. The reason for this is that the modified quadrature formula is numerically more stable.

4.2. Numerical Test Results

To test the method, we examined all of the Laplace transforms that are used in the overview article by Davies and Martin (cf. [12]). In this subsection we discuss the results for eight analytical test functions. These results are presented in Table 1. The inversions are done in 32 points and so $M = 32$. We have taken $M_2 = 8M = 256$, $a = 44/M_2$, and $n = 16$. The computations are done with double precision. We have taken $\Delta = 1/16$, $\Delta = 1$, and $\Delta = 10$. We see that for smooth functions the approximation error seems to be independent of Δ. The reason for this is that the approx-

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imation error is dominated with round-off error. From all of the examples, we can conclude that the method is very accurate, robust, and fast. In Section 6.2 we discuss the other test functions that are used in the overview article by Davies and Martin (cf. [12]).

5. MULTIDIMENSIONAL LAPLACE TRANSFORM

Let f be a complex-valued Lebesgue integrable function with $e^{-(c_1 x + c_2 y)} f(x,y) \in L^1(\mathbb{R}^2_+)$. The two-dimensional Laplace transform of f is defined by the integral

$$\hat{f}(s,r) := \int_0^\infty \int_0^\infty e^{-(sx+ry)} f(x,y)\, dx\, dy, \qquad \operatorname{Re}(s) > c_1, \operatorname{Re}(r) > c_2. \tag{5.1}$$

In order to extend the algorithm of Section 4 to a two-dimensional Laplace transform algorithm, we need the two-dimensional Poisson summation formula (PSF2).

THEOREM 5.1 (PSF2): *If $f \in L^1(\mathbb{R}^2_+)$ and f is of bounded variation, then for all v and $\omega \in [0,1)$,*

$$\hat{G}_{ab}(v,\omega) = G_{ab}(v,\omega), \tag{5.2}$$

where

$$\hat{G}_{ab}(v,\omega) = \sum_{k=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \hat{f}(a + 2\pi i(k+v), b + 2\pi i(j+\omega)) \tag{5.3}$$

and

$$G_{ab}(v,\omega) = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} e^{-ak} e^{-bj} e^{-i2\pi k v} e^{-i2\pi j \omega} f(k,j);$$

here, $f(x,y)$ has to be understood as

$$\frac{f(x^+,y^+) + f(x^+,y^-) + f(x^-,y^+) + f(x^-,y^-)}{4}.$$

Similarly as in the one-dimensional case, we associate with (5.3) an inner product; we call this inner product $\langle \cdot,\cdot \rangle_{Q_{v\omega}}$.

DEFINITION 5.2: *Let the inner product $\langle \cdot,\cdot \rangle_{Q_{v\omega}}$ be given by*

$$\langle f,g \rangle_{Q_{v\omega}} = \sum_{k,j} |u_k^v|^2 |u_j^\omega|^2 f(u_k^v, u_j^\omega) g^*(u_k^v, u_j^\omega),$$

where $u_k^v = 1/(2\pi i(k+v))$.

Having $\mathbf{1}(s,r) = 1$ and $\Psi\hat{f}(s,r) = s^{-1} r^{-1} \hat{f}(s^{-1}, r^{-1})$, we can write (5.3) as $\langle \Psi\hat{f}, \Psi\mathbf{1} \rangle_{Q_{v\omega}}$. The idea is to approximate this inner product with a Gaussian quadrature rule. Similarly as in the one-dimensional case, we associate with the inner

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product $\langle \cdot,\cdot \rangle_{Q_{\upsilon\omega}}$ the norm $\|\cdot\|_{Q_{\upsilon\omega}}$ and introduce the sequence space $L^2(Q_{\upsilon\omega})$. We say that a function f belongs to $L^2(Q_{\upsilon\omega})$ iff the sequence $\{f(u_k^\upsilon, u_j^\omega)\}$ belongs to $L^2(Q_{\upsilon\omega})$. Let the polynomials $\{q_{kj}^{\upsilon\omega}\}$ be given by

$$q_{kj}^{\upsilon\omega}(s,r) = q_k^\upsilon(s) q_j^\omega(r).$$

The following result holds.

THEOREM 5.3: *The set* $\{q_{kj}^{\upsilon\omega}; j = 0,1,\ldots\}$ *is a complete orthogonal set of polynomials in* $L^2(Q_{\upsilon\omega})$.

The proof is given in Appendix E.

We can now easily obtain the desired Gaussian quadrature rule. We denote this quadrature rule by $\langle \cdot,\cdot \rangle_{Q_{\upsilon\omega}^n}$.

DEFINITION 5.4: *The inner product* $\langle \cdot,\cdot \rangle_{Q_{\upsilon\omega}^n}$ *is given by*

$$\langle f, g \rangle_{Q_{\upsilon\omega}^n} = \sum_{k=1}^n \sum_{j=1}^n \alpha_k^\upsilon \alpha_j^\omega \hat{f}(\mu_k^\upsilon, \mu_j^\omega) \hat{g}^*(\mu_k^\upsilon, \mu_j^\omega). \tag{5.4}$$

The $\{\mu_k^\upsilon\}$ *are the zeros of the polynomial* q_n^υ*. The so-called Christophel numbers* $\{\alpha_k\}$ *are positive numbers given by*

$$\alpha_k^\upsilon = \frac{1}{\sum_{j=1}^n |q_j^\upsilon(u_k^\upsilon)|^2}.$$

Having $\mathbf{1}(s,r) = 1$ and $\Psi\hat{f}(s,r) = s^{-1}r^{-1}\hat{f}(s^{-1}, r^{-1})$, we approximate $\langle \Psi\hat{f}, \mathbf{1} \rangle_{Q_{\upsilon\omega}}$ with Gaussian quadrature rule (5.4). By considering the real part of the quadrature formula, we obtain

$$\begin{aligned} \tilde{F}_{ab}(\upsilon,\omega) &\approx \sum_{k=-\infty}^{\infty} \sum_{j=-\infty}^{\infty} \mathrm{Re}(\hat{f}(a + 2\pi i(k+\upsilon), b + 2\pi i(j+\omega))) \\ &= \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} e^{-ak} e^{-jb} \cos(i 2\pi(k\upsilon + j\omega)) f(k,j), \end{aligned} \tag{5.5}$$

with

$$\tilde{F}_{ab}(\upsilon,\omega) = \sum_{k=1}^n \sum_{j=1}^n \beta_{kj}^{\upsilon\omega} \mathrm{Re}\left(\hat{f}\left(a + \frac{1}{\mu_k^\upsilon}, b + \frac{1}{\mu_k^\omega}\right)\right),$$

where

$$\beta_{kj}^{\upsilon\omega} = \frac{\alpha_k^\upsilon}{|\mu_k^\upsilon|^2} \frac{\alpha_j^\omega}{|\mu_j^\omega|^2}.$$

The second equation in (5.5) follows from PSF2 (cf. (5.2)).

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As in Section 4, we approximate quadrature rule (5.5) with a numerically more stable quadrature rule. Again, we start by writing the PSF2 (cf. (5.1)) as

$$\hat{H}_{ab}(v,\omega) = H_{ab}(v,\omega),$$

where

$$\hat{H}_{ab}(v,\omega) = \sum_{k=-\infty}^{\infty}\sum_{j=-\infty}^{\infty} \mathrm{Re}(\hat{f}(\rho_v^a + i(2k+1)\pi, \rho_v^b + i(2j+1)\pi)), \tag{5.6}$$

with

$$\rho_v^a = a + 2\pi i\left(v - \frac{1}{2}\right) \quad \text{and} \quad \rho_v^b = b + 2\pi i\left(v - \frac{1}{2}\right),$$

and

$$H_{ab}(v,\omega) = \sum_{k=0}^{\infty}\sum_{j=0}^{\infty} e^{-ak}e^{-jb}\cos(i2\pi(kv + j\omega))f(k,j).$$

Applying the quadrature rule to (5.6) yields the approximation

$$F_{ab}(v,\omega) \approx \hat{H}_{ab}(v,\omega) = H_{ab}(v,\omega), \tag{5.7}$$

with

$$F_{ab}(v,\omega) = \sum_{k=1}^{n}\sum_{j=1}^{n} \beta_{kj}\,\mathrm{Re}(\hat{f}(i\lambda_k + a + 2\pi i v, i\lambda_j + b + 2\pi i\omega)),$$

where

$$\lambda_k = \frac{1}{i\mu_k^{0.5}} - \pi \quad \text{and} \quad \beta_{kj} = \frac{\alpha_k^{0.5}}{|\mu_k^{0.5}|^2}\,\frac{\alpha_j^{0.5}}{|\mu_j^{0.5}|^2}.$$

We make F_{ab} periodic by defining

$$\tilde{F}_a(0,\omega) = \tilde{F}_a(1,\omega) = \frac{1}{2}\,(F_a(0,\omega) + F_a(1,\omega)),$$

$$\tilde{F}_a(v,0) = \tilde{F}_a(v,1) = \frac{1}{2}\,(F_a(v,0) + F_a(v,1))$$

and by defining $\tilde{F}_a(0,0)$, $\tilde{F}_a(0,1)$, $\tilde{F}_a(1,0)$, and $\tilde{F}_a(1,1)$ all equal to

$$\frac{1}{4}\,(F_a(0,0) + F_a(0,1) + F_a(1,0) + F_a(1,1)).$$

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It remains to compute the function values $f(k,j)$, $k = 0,1,\ldots,M_1 - 1$ and $j = 0, 1,\ldots,M_2 - 1$. We can realize this by the discrete Fourier series inversion formula

$$\frac{e^{ak}}{N_1}\frac{e^{bj}}{N_2}\sum_{l=0}^{N_1-1}\sum_{m=0}^{N_2-1}\cos\left(2\pi\left(\frac{kl}{N_1}+\frac{jm}{N_2}\right)\right)\tilde{F}_{ab}\left(\frac{l}{N_1},\frac{m}{N_2}\right), \tag{5.8}$$

where N_1 and N_2 are given powers of 2. With the well-known (two-dimensional) FFT algorithm (cf. Cooley and Tukey [11]), we can compute the sums (5.8) in $N_1 N_2 \log(N_1 N_2)$ time.

Algorithm

Input: $\hat{f}$, Δ_1, Δ_2, M_1, and M_2 with M_1 and M_2 powers of 2
Output: $f(\ell\Delta_1, m\Delta_2)$, $\ell = 0,1,\ldots,M_1 - 1$, $m = 0,1,\ldots,M_2 - 1$
Parameters: $N_1 = 8M_1$, $N_2 = 8M_2$, $a = 44/N_1$, $b = 44/N_2$, and $n = 16$

Step 1. For $k = 0,1,\ldots,N_1$, $j = 1,2,\ldots,n$, $m = 0,1,\ldots,N_2$, and $l = 1,2,\ldots,n$, compute the numbers

$$\hat{f}_{jklm} = \operatorname{Re}\left[\hat{f}\left(\frac{1}{\Delta_1}\left(a + i\lambda_j + \frac{2i\pi k}{N_1}\right), \frac{1}{\Delta_2}\left(b + i\lambda_l + \frac{2i\pi m}{N_2}\right)\right)\right],$$

and the numbers

$$\hat{f}_{km} = \frac{1}{\Delta_1}\frac{1}{\Delta_2}\sum_{j=1}^{n}\sum_{l=1}^{n}\beta_{jl}\hat{f}_{jklm}.$$

Set

$$\hat{f}_{0m} = \frac{1}{2}(\hat{f}_{0m} + \hat{f}_{N_1 m}), \qquad \hat{f}_{k0} = \frac{1}{2}(\hat{f}_{k0} + \hat{f}_{kN_2}),$$

$$\hat{f}_{00} = \frac{1}{4}(\hat{f}_{00} + \hat{f}_{N_1 0} + \hat{f}_{0N_2} + \hat{f}_{N_1 N_2}).$$

Step 2. For $\ell = 0,1,\ldots,N_1 - 1$ and $m = 0,1,\ldots,N_2 - 1$, compute the numbers

$$f_{\ell m} = \frac{1}{N_1}\frac{1}{N_2}\sum_{k=0}^{N_1-1}\sum_{j=0}^{N_2-1}\hat{f}_{kj}\cos\left(\frac{2\pi\ell k}{N_1} + \frac{2\pi m j}{N_2}\right)$$

with the backwards FFT algorithm.

Step 3. Set $f(\ell\Delta_1, m\Delta_2) = e^{a\ell}e^{bm}f_{\ell m}$ for $\ell = 0,1,\ldots,M_1 - 1$ and $m = 0, 1,\ldots,M_2 - 1$.

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Remark 5.5: We can compute the function values $f(k\Delta_1, j\Delta_2)$, $k,j = 0,1,\ldots,$ by applying the quadrature rule to the scaled Laplace transform

$$\hat{f}_{\Delta_1,\Delta_2}(s,r) = \frac{1}{\Delta_1}\frac{1}{\Delta_2}\hat{f}\left(\frac{s}{\Delta_1}, \frac{r}{\Delta_2}\right).$$

Remark 5.6: In a similar way, we can invert higher-dimensional transforms and compute the function values $f(k_1\Delta_1,\ldots,k_d\Delta_d)$, $k_j = 0,1,\ldots,M_j - 1$, at once in $\prod_{j=1}^{d} M_j \log(\prod_{j=1}^{d} M_j)$ time.

Remark 5.7: We have tested the two-dimensional Laplace transform inversion with many numerical experiments. All of these experiments show that the two-dimensional inversion algorithm is extremely accurate for smooth functions. In Section 6 we discuss the number of modifications to obtain the same accurate results for nonsmooth functions. We discuss them in the context of the one-dimensional inversion algorithm. The modifications can also be used in combination with the two-dimensional Laplace transform inversion algorithm.

6. MODIFICATIONS FOR NONSMOOTH FUNCTIONS

In Appendix G we prove that the inversion algorithm is extremely accurate for smooth functions. In the following subsections we present a number of modifications to obtain the same accurate results for nonsmooth functions. In Section 6.1 we discuss a modification for piecewise smooth functions. With this modification, we can obtain results near machine precision for functions with discontinuities in the points $k\Delta$, $k \in \mathbb{Z}$. In Section 6.2 we discuss a modification for functions with singularities at arbitrary locations. With this modification, we can obtain results near machine precision for functions with discontinuities at arbitrary but a priori known locations. In Section 6.3, we discuss a modification that is effective for almost all kinds of discontinuity, singularity, and local nonsmoothness. With this modification, we can obtain results near machine precision in continuity points for almost all functions, even if we do not know the discontinuities and singularities a priori. The modifications of the next subsections can, in principle, also be used in combination with other Fourier series methods. The effectiveness of the modifications in combination with other Fourier series methods is a subject for future research.

6.1. Piecewise Smooth Functions

In this subsection we discuss a modification for piecewise smooth functions. With this modification, we can obtain results near machine precision for functions with discontinuities in the points $k\Delta$, $k \in \mathbb{Z}$. The discontinuities of such a function are represented as exponentials in the Laplace transform. To be more precise, suppose that the function f is a piecewise smooth function with discontinuities in the points k, $k \in \mathbb{Z}$. We can write the Laplace transform $\hat{f}$ as

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$$\hat{f}(s) = V(s, e^{-s}) = \sum_j e^{-js}\hat{f}_j(s),$$

with $\hat{f}_j$ the Laplace transforms of functions that are smooth on $[0,\infty)$. The function f is then given by

$$f(t) = \sum_j f_j(t-j);$$

here, we use the translation property. Since the f_j are smooth functions on $[0,\infty)$, the quadrature rule is accurate. Hence,

$$\sum_{k=1}^{n} \beta_k e^{-j(a+2\pi iv)}\hat{f}_j(i\lambda_k + s_v^a) \approx \sum_{k=0}^{\infty} e^{-a(k+j)}e^{-i2\pi(k+j)v}f_j(k)$$

$$= \sum_{k=j}^{\infty} e^{-ak}e^{-i2\pi kv}f_j(k-j),$$

with $s_v^a = a + 2\pi iv$. On the other hand,

$$\sum_j \sum_{k=1}^{n} \beta_k e^{-j(a+2\pi iv)}\hat{f}_j(i\lambda_k + s_v^a) = \sum_{k=1}^{n}\sum_j \beta_k e^{-j(a+2\pi iv)}\hat{f}_j(i\lambda_k + s_v^a)$$

$$= \sum_{k=1}^{n} \beta_k V(i\lambda_k + s_v^a, e^{-a+2\pi iv}).$$

Combining the above equations yields

$$\sum_{k=0}^{\infty} e^{-ak}e^{-i2\pi kv}f(k) \approx \sum_{k=1}^{n} \beta_k V(i\lambda_k + s_v^a, e^{-a-2\pi iv}).$$

We now proceed as in Section 4 and compute the function values $f(k)$, $k = 0, 1, \ldots, M-1$, with

$$\frac{e^{ak}}{M_2}\sum_{j=0}^{M_2-1} \cos\left(\frac{2\pi jk}{M_2}\right)F_a\left(\frac{j}{M_2}\right),$$

where

$$F_a(v) = \sum_{k=1}^{n} \beta_k \mathrm{Re}(V(i\lambda_k + a + 2\pi iv, e^{-a-2\pi iv})).$$

Remark 6.1: If f is piecewise smooth, with discontinuities in the points $k\alpha$, $k \in \mathbb{Z}$, we can write the Laplace transform $\hat{f}$ as $\hat{f}(s) = V(s, e^{-s\alpha})$. We scale the Laplace transform to

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$$\frac{m}{\alpha}\hat{f}\left(\frac{sm}{\alpha}\right) = \frac{m}{\alpha}V\left(\frac{sm}{\alpha}, e^{-sm}\right)$$

and can obtain the values $\{f(k\alpha/m)\}$ with high precision.

As an example, consider the Laplace transform

$$\hat{f}(s) := \frac{e^{-s}}{s}.$$

We then obtain the quadrature formula

$$\sum_{k=1}^{n} \beta_k \operatorname{Re}\left(\frac{e^{-am}e^{-i2\pi m v}}{a + i\lambda_k + 2\pi i v}\right).$$

Algorithm

Input: V: $f(s) = \hat{V}(s, e^{-s\Delta})$, Δ, and M, with M a power of 2
Output: $f(\ell\Delta)$, $\ell = 0,1,\ldots,M-1$
Parameters: $M_2 = 8M$, $a = 44/M_2$, and $n = 16$

Step 1. For $k = 0,1,\ldots,M_2$ and $j = 1,2,\ldots,n$, compute the numbers

$$\hat{f}_{jk} = \operatorname{Re}\left[V\left(\frac{1}{\Delta}\left(a + i\lambda_j + \frac{2i\pi k}{M_2}\right), \exp\left(-\left(a + \frac{2i\pi k}{M_2}\right)\right)\right)\right]$$

and the numbers

$$\hat{f}_k = \frac{1}{\Delta}\sum_{j=1}^{n} \beta_j \hat{f}_{jk} \quad \text{and} \quad \hat{f}_0 = \frac{\hat{f}_0 + \hat{f}_{M_2}}{2}.$$

Step 2. For $\ell = 0,1,\ldots,M_2 - 1$, compute the numbers

$$f_\ell = \frac{1}{M_2}\sum_{k=0}^{M_2-1} \hat{f}_k \cos\left(\frac{2\pi\ell k}{M_2}\right)$$

with the backwards FFT algorithm.

Step 3. Set $f(\ell\Delta) = e^{a\ell} f_\ell$ for $\ell = 0,1,\ldots,M-1$.

In Appendix H we discuss the details of Steps 2 and 3 of the algorithm.

We test this modification on two discontinuous test functions. The results are presented in Table 2. The inversions are done in 32 points and so $M = 32$. We have taken $M_2 = 256 = 8M$ and $\Delta = 1/16$ and we have taken $a = 44/M_2$. In addition to the choice of the previous parameters, we have taken $n = 16$.

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TABLE 2. Results for Noncontinuous Test Functions

No.	Function	Laplace Transform	MAE
17	$H(t-1)$	$s^{-1}\exp(-s)$	2e-15
18	Square wave	$s^{-1}(1+\exp(-s))^{-1}$	8e-15

Note: The mean absolute error (MAE) is presented for the inversion of two noncontinuous functions in the points 0,1/16,…,31/16. We have used the modification of Section 6.1. From this table, we can conclude that for noncontinuous functions the results are also very accurate. We mention that, even in the discontinuity points, we have a precision of 15 digits.

We can conclude that our method is also very accurate, robust, and fast for discontinuous functions. In the next subsection we show the effectiveness of the modification of this subsection with an application from queuing theory.

6.1.1. An application in queuing theory. Consider the $M/G/1$ queue arrival rate λ and general service time distribution B with first moment μ_B. It is assumed that $\rho = \lambda\mu_B < 1$. It is well known that the distribution of the stationary waiting time $\mathbf{W}$ is given by (see, e.g., Asmussen [6])

$$W(x) := P\{\mathbf{W} \le x\} = (1-\rho)\sum_{n=0}^{\infty} \rho^n B_0^{*n}(x), \tag{6.1}$$

with $B_0(x) = (1/\mu_B)\int_0^x (1-B(t))\,dt$. The Laplace transform $\hat{W}$ of W is given by

$$\hat{W}(s) = \frac{1}{s}\frac{1-\rho}{1-\rho\left(\dfrac{1-\hat{B}(s)}{s\mu_B}\right)}. \tag{6.2}$$

As an example, consider the $M/D/1$ queue; that is, the service times are deterministic, with mean 1. For this case, the Laplace transform $\hat{W}$ is given by

$$\hat{W}(s) = \frac{1}{s}\frac{1-\rho}{1-\rho(1-e^{-s})/s}. \tag{6.3}$$

Observe that $\hat{W}(s)$ contains the factor $\exp(-s)$. Therefore, introduce the function

$$V(s,z) = \frac{1}{s}\frac{1-\rho}{1-\rho(1-z)/s}. \tag{6.4}$$

For this choice, it follows that $\hat{W}(s) = v(s,\exp(-s))$ and, therefore, we can apply the modification of Section 6.1. We have calculated the waiting time distribution for $\rho = 0.7$, 0.8, 0.9, and 0.95. By comparing our results with results of the algo-

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TABLE 3. Results for the Waiting Time Distribution in the $M/D/1$ Queue

ρ	MAE
0.7	3e-14
0.8	5e-14
0.9	8e-14
0.95	1e-13

Note: The mean absolute error (MAE) is presented for the inversion of the Laplace transform of the limited distribution of the waiting time in an $M/D/1$ queue. We have taken $\rho = 0.7$, 0.8, 0.9, and 0.95. We have calculate the values $W(k), k = 0,1,\ldots,63$. We have taken $\Delta = 1$, $n = 16$ and $a = 44/M_2$.We used the modification of Section 6.1.

rithm in Tijms [26, p. 381], it appears that we can calculate the waiting time distribution with near machine accuracy in a fraction of a second; see Table 3.

Remark 6.2: We can generalize the above approach to a service distribution

$$D(x) = \sum_{k=1}^{\infty} p_k \mathbf{1}_{\{x \le k\}}.$$

We then obtain

$$V(s,z) = \frac{1}{s} \frac{1-\rho}{1-\rho\left(1-\sum_{k=0}^{\infty} p_k z^k\right)/s}.$$

6.2. Functions with Singularities

In this subsection we discuss a modification for functions with singularities at arbitrary locations. With this modification, we can obtain results near machine precision for functions with discontinuities at arbitrary but a priori known locations. Suppose that there is a singularity in $t = \alpha$, with $\alpha \in \mathbb{R}$. We then consider the function

$$f_w(x) := w(x)^q f(x), \tag{6.5}$$

where the so-called window function w is a trigonometric polynomial with period 1, $w(0) = 1$, and $w(\alpha) = 0$, and q is a positive integral number. Hence, the function f_w is smooth in $t = \alpha$ and

$$f_w(k) = f(k),\ k = 0,1,\ldots.$$

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We can compute the function values $f(k)$ by inverting the Laplace transform $\hat{f}_w$ with the algorithm of Section 4. The following class of window functions gives results near machine precision:

$$\begin{aligned} w(x) &= \left(\cos(p\pi x) - \frac{\cos(p\pi\alpha)}{\sin(p\pi\alpha)}\sin(p\pi x)\right)^2 \\ &= (Ae^{ip\pi x} + Be^{-ip\pi x})^2, \qquad p \in \mathbb{N}, \end{aligned}$$

where the coefficients A and B are given by

$$A = \left(\frac{1}{2} - \frac{1}{2i}\frac{\cos(p\pi\alpha)}{\sin(p\pi\alpha)}\right) \quad \text{and} \quad B = \left(\frac{1}{2} + \frac{1}{2i}\frac{\cos(p\pi\alpha)}{\sin(p\pi\alpha)}\right)$$

and p is chosen such that $(p\alpha \bmod 1)$ is close to $\frac{1}{2}$. We obtain by the modulation property that

$$\hat{f}_w(s) = \sum_{k=0}^{2q} \binom{2q}{k} A^{2q-k} B^k \hat{f}(s + 2\pi p(q-k)).$$

Remark 6.3: Suppose that there are singularities in the points α_j, $j = 1,2,\ldots,m$. Then we can multiply the windows; that is, we take

$$w(x) = \prod_{j=1}^{m} w_j^q(x),$$

where w_j is a trigonometric polynomial with period 1, $w_j(0) = 1$, and $w_j(\alpha_j) = 0$.

Remark 6.4: If we want to compute $f(k\Delta)$, we have to replace $\hat{f}_w$ with $(1/\Delta)\hat{f}_w(s/\Delta)$.

If there is a singularity in $t = 0$, then A and B are not defined. Consider, therefore, the function

$$w(x) = \sin^2\left(\frac{\pi x}{2}\right). \tag{6.6}$$

The function w has period 2, $w(1) = 1$, $w(\alpha) = 0$, and $\partial w(\alpha)/\partial\alpha = 0$. Hence, f_w is smooth in $t = 0$ and

$$f_w(2k+1) = f(2k+1), \qquad k = 0,1,\ldots.$$

We obtain from

$$\begin{aligned} \left(\sin\left(\frac{\pi x}{2}\right)\right)^{2q} &= \left(\frac{e^{i(\pi/2)x} - e^{-i(\pi/2)x}}{2i}\right)^{2q} \\ &= \left(\frac{1}{2}\right)^{2q} \sum_{k=0}^{2q} \binom{2q}{k} (-1)^{q-k} e^{-i\pi(q-k)x} \end{aligned}$$

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and the modulation property that

$$\hat{f}_w(s) = \left(\frac{1}{2}\right)^{2q} \sum_{k=0}^{2q} \binom{2q}{k} (-1)^{q-k} \hat{f}_q(s + i\pi(q-k)).$$

We can compute the function values $f(2k+1)$, with the algorithm of Section 4. If we want to compute $f(\Delta(2k+1))$, we have to replace $\hat{f}_w$ with $(1/\Delta)\hat{f}_w(s/\Delta)$.

Remark 6.5: For singularities at $t = 0$ of the order x^α, $0 < \alpha < 1$, we can obtain with $q = 1$ results near machine precision. For singularities at $t = 0$ of the order x^α, $-1 < \alpha < 0$, with $q = 2$ we can obtain results near machine precision. For discontinuities and singularities at arbitrary t, we recommend using $q = 6$.

Remark 6.6: Since the composite inverse function $f_w(t\Delta)$ is a highly oscillating function, we recommend choosing $n = 32$. With this choice, we obtain results near machine precision. If the inversion point is close to a singularity, we can compute $f(t)$ accurately by inverting the scaled Laplace transform

$$f_w(t) = w(t) f(\Delta t),$$

with Δ small enough. The price we have to pay for a small Δ is that M becomes large ($M \approx t/\Delta$).

Remark 6.7: The idea of smoothing through the use of multiplying smoothing functions has been discussed in the context of Euler summation by O'Cinneide [17] and Sakurai [21]. O'Cinneide called the idea "product smoothing."

We end this subsection with the results for eight test functions with singularities that were in the overview article of Davies and Martin (cf. [12]). These results are presented in Table 4. The inversions are done in 32 points and so $M = 32$. We have taken $M_2 = 256 = 8M$, and for all of the examples, we have taken $a = 44/M_2$. We have used the window function $w(t) = \sin(\pi t/2)^2$, and we have taken q according to Remark 6.5. In addition to the choice of the previous parameters, we have taken $n = 32$. The computations are done with double precision. We have taken $\Delta = 1/16$, $\Delta = 1$, and $\Delta = 10$. We see that, for smooth functions, the approximation error seems to be independent of Δ. The reason for this is that the approximation error is dominated with round-off errors and the error caused by the oscillation of the window function.

From all of the examples, we can conclude that the method is very accurate, robust, and fast for functions with singularities.

6.3. A Robust Laplace Inversion Algorithm

In this subsection we discuss a modification that is effective for almost all kinds of discontinuity, singularity, and local nonsmoothness. With this modification, we can obtain results near machine precision in continuity points for almost all functions, even if we do not know the discontinuities and singularities a priori. As in Sec-

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Table 4. Results for Continuous Nonanalytical Test Functions

No.	Function	Laplace Transform
9	$(\pi x)^{-1/2}\cos(2x^{1/2})$	$s^{-1/2}\exp(-s^{-1})$
10	$(\pi x)^{-1/2}$	$s^{-1/2}$
11	$-\gamma - \ln(x)$	$s^{-1}\ln(s)$
12	$(e^{-x/4} - e^{-x/2})(4\pi x^3)^{-1/2}$	$(s+\frac{1}{2})^{1/2} - (s+\frac{1}{4})^{1/2}$
13	$2e^{-4/x}(\pi x^3)^{-1/2}$	$\exp(-4s^{1/2})$
14	$\sin(x)/x$	$\arctan(1/s)$
15	$x^{1/3}$	$\Gamma(\frac{4}{3})s^{-4/3}$
16	$x^{1/4}$	$\Gamma(\frac{5}{4})s^{-5/4}$

No.	$\Delta = 1/16$	$\Delta = 1$	$\Delta = 10$
9	3e-14	8e-15	3e-15
10	1e-14	4e-15	4e-15
11	2e-15	1e-14	2e-14
12	3e-15	8e-16	4e-16
13	3e-16	4e-16	1e-14
14	1e-14	1e-15	7e-16
15	9e-15	1e-14	2e-14
16	8e-15	1e-14	2e-14

Note: In the table the mean absolute error $\sum_{k=0}^{M-1} e(\Delta(2k+1))/(1+e(\Delta(2k+1)))$ is presented for the inversion of eight functions with singularities in $x = 0$. We have computed the function values in the points $\{1/16, 3/16, \ldots, 63/16\}, \{1, 3, \ldots, 63\}$, and $\{10, 30, \ldots, 630\}$.

tion 6.2, we compute the function value $f(k)$ by inverting the Laplace transform of the function

$$f_{w_k}(t) = w_k(t)f(t),$$

but now the window function depends on the point k; that is, for the computation of each function value $f(k)$ we use a different window function. We choose the window function such that the ϵ-support $\{t; |e^{-\alpha t}f_{w_k}(t)| \geq \epsilon\}$ of f_{w_k} is contained in $[k-\delta, k+\delta]$, with δ given positive control parameters, ϵ a given tolerance, and $w_k(k) = 1$. The advantage of this construction is that it is sufficient that the function f is smooth on $[k-\delta, k+\delta]$, in order that the function f_{w_k} is smooth on $[0,\infty)$. Thus, we only need that the function f is smooth on $[k-\delta, k+\delta]$ to compute $f(k)$ accurately with the quadrature rule. Hence, we can obtain results near machine precision in continuity points for almost all functions.

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A second advantage is that we can efficiently invert the resulting z-transform. As the ϵ-support of f_{w_k} is contained in $[k-\delta, k+\delta]$ implies that

$$\sum_{j=1}^{n} \beta_j \operatorname{Re}(\hat{f}_{w_k}(i\lambda_j + 2\pi i v + a)) \approx \sum_{j=0}^{\infty} w_k(j) f(j) e^{-ja} \cos(2\pi j v)$$

$$= \sum_{j \in [k-\delta, k+\delta]} w_k(j) f(j) e^{-ja} \cos(2\pi j v)$$

(the first equation follows from (4.5)) and the N-point discrete Fourier transform computes the numbers

$$\tilde{f}_k = \sum_j f_{k+jN}$$

(cf. Appendix H), we can compute the function values $f(k)$ efficiently with an N-point discrete Fourier transform ($N \geq 1 + 2\lfloor\delta\rfloor$).

We can construct the window functions with the desired properties as follows: Let w be a smooth bounded function satisfying

$$|w(t)| \leq \epsilon, \qquad t \in [-P/2, -\delta] \cup [\delta_u, P/2], \qquad w(0) = 1,$$

with P a given positive number. We choose the damping factor α such that

$$|e^{-\alpha t} f(t)| \leq \frac{\epsilon}{\sup_{x \in [-P/2, P/2]} |w(x)|} \quad \text{for } t > P. \tag{6.7}$$

We extend w to a periodic function with period P by setting

$$w(t + kP) = w(t), \qquad t \in [-P/2, P/2), \quad \text{and} \quad k \in \mathbb{Z}.$$

The desired window function w_k is defined by

$$w_k(t) = w(t-k).$$

We will now show how we can efficiently evaluate the Fourier series F_k,

$$F_k(v) = \sum_{j=1}^{n} \beta_j \operatorname{Re}(\hat{f}_{w_k}(i\lambda_j + 2\pi i v))$$

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for $k = 0, 1, \ldots, M-1$. Since w has period P and w is smooth, we can expand w in a fast converging Fourier series. Thus, we can write

$$w_k(t) = w(t-k) = \sum_{j=-\infty}^{\infty} e^{2\pi ijk/P} A_j e^{-2\pi ijt/P},$$

with

$$A_j = \frac{1}{P}\int_{-P/2}^{P/2} w(t) e^{2\pi ijt/P}\, dt.$$

This yields that the Laplace transform of f_{w_k} is given by

$$\hat{f}_{w_k}(s) = \sum_{j=-\infty}^{\infty} e^{2\pi ijk/P} A_j \hat{f}\left(s + \frac{2\pi ij}{P} + a\right). \tag{6.8}$$

Since w is a smooth periodic function, the $\{A_j\}$ converge rapidly to zero. Hence, we can approximate $\hat{f}_{w_k}$ accurately with

$$\hat{f}_{w_k}(s) = \sum_{j=-J}^{J} e^{2\pi ijk/P} A_j \hat{f}\left(s + \frac{2\pi ij}{P} + a\right), \tag{6.9}$$

for J large enough. Hence,

$$F_k(v) = \mathrm{Re}\left(\sum_{j=-J}^{J} e^{2\pi ijk/P} A_j G\left(v + \frac{j}{P}\right)\right),$$

with

$$G(v) = \sum_{k=1}^{n} \beta_k \hat{f}(a + \lambda_k + 2\pi iv).$$

Moreover, if J is a multiple of P, then

$$F_k(v) = \mathrm{Re}\left(\sum_{l=0}^{P-1} e^{2\pi ilk/P} \sum_{m=-L}^{L-1} A_{mP+l} G\left(v + m + \frac{l}{P}\right)\right), \tag{6.10}$$

with $L = J/P$. We make F_k periodic by defining $F_k(0)$ and $F_k(1)$ equal to

$$\frac{1}{2}\left(F_k(0) + F_k(1)\right).$$

We can compute the sums (6.10) in $L\log(L) + J$ time with the FFT algorithm (cf. Cooley and Tukey [11]). It remains to compute the function values $f(k)$, $k = 0, 1, \ldots, M-1$. We can realize this by the discrete Fourier series inversion formula

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$$f(k) \approx \frac{e^{\alpha k}}{\hat{m}} \sum_{j=0}^{\hat{m}-1} \cos\left(\frac{2\pi jl}{\hat{m}}\right) F_k\left(\frac{j}{\hat{m}}\right),$$

with $\hat{m} = 1 + 2\lfloor \delta \rfloor$ and $l = k \bmod(\hat{m})$. If $\delta \leq 1$, then

$$f(k) \approx (-1)^k e^{\alpha k} F_k\left(\frac{1}{2}\right).$$

Let us finally define the window function w. A good choice is the so-called Gaussian window (cf. Mallat [15]). The Gaussian window is defined by

$$w(t) = \exp\left(-\frac{1}{2}\left(\frac{t}{\sigma}\right)^2\right),$$

with σ a given scale parameter. Given a prespecified tolerance ϵ, the scale parameter σ is chosen such that

$$\exp\left(-\frac{1}{2}\left(\frac{\delta}{\sigma}\right)^2\right) < \epsilon. \tag{6.11}$$

We can compute the numbers A_j by

$$\frac{1}{P}\int_{-P/2}^{P/2} \exp\left(-\frac{1}{2}\left(\frac{t}{\sigma}\right)^2\right) e^{2\pi ijt/P}\, dt \approx \frac{1}{P}\int_{-\infty}^{\infty} \exp\left(-\frac{1}{2}\left(\frac{t}{\sigma}\right)^2\right) e^{2\pi ijt/P}\, dt$$
$$= \frac{\sigma\sqrt{2\pi}}{P} \exp\left(-\frac{1}{2}\left(\frac{2\pi j}{P}\right)^2 \sigma^2\right).$$

The truncation parameter L (in (6.10)) is chosen as

$$L = \arg\min\left\{L : \frac{\sigma\sqrt{2\pi}}{P} \exp\left(-\frac{1}{2}(2\pi L)^2\sigma^2\right) < \epsilon\right\} \tag{6.12}$$

and δ is chosen as $\delta = 1$.

Algorithm

Input: $\hat{f}$, ϵ (desired precision), Δ, and M, with M a power of 2
Output: $f(\ell\Delta)$, $\ell = 0, 1, \ldots, M-1$
Parameters: $P = 8M$, $\delta = 1$, L (cf. (6.12)), σ (cf. (6.11)), and $n = 48$

Step 1. For $k = -PL, \ldots, PL - 1$ and $j = 1, 2, \ldots, n$, compute the numbers

$$\hat{f}_{jk} = \mathrm{Re}\left[\hat{f}\left(\frac{a + i\lambda_j + i\pi + \dfrac{2i\pi k}{P}}{\Delta}\right)\right],$$

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for $k = -PL, \ldots, PL-1$, compute the numbers

$$\hat{f}_k = \frac{1}{\Delta} \sum_{j=1}^{n} \beta_j \hat{f}_{jk},$$

and for $j = 0, 1, \ldots, P-1$, compute the numbers

$$\hat{g}_j = \sum_{m=-L}^{L-1} A_{mP+j} \hat{f}_{mP+j},$$

with

$$A_j = \frac{\sigma\sqrt{2\pi}}{P} \exp\left(-\frac{1}{2}\left(\frac{2\pi j}{P}\right)^2 \sigma^2\right).$$

Step 2. Compute $f_k = \mathrm{Re}(\sum_{j=0}^{P-1} e^{2\pi ijk/P} \hat{g}_j)$, for $k = 0, 1, \ldots, P-1$, with the FFT algorithm.

Step 3. Compute $f(k\Delta)$ with $f(k\Delta) = (-1)^k e^{ak} f_k$, for $k = 0, 1, \ldots, M-1$.

Remark 6.8: The composite inverse functions f_{w_k} are highly peaked; therefore we recommend choosing $n = 48$. With this choice, we obtain results near machine precision.

Remark 6.9: For an arbitrary window function, we can also compute the coefficients A_j efficiently with the fractional FFT (cf. [7]). Since $|w(t)| < \epsilon$ for $[-P/2, -\delta_l] \cup [\delta_u, P/2]$, we can write this discrete Fourier transform as

$$A_j \approx \frac{1}{PN} \sum_{k=-P}^{P} w\left(\frac{k}{N}\right) e^{(2\pi ij/P)(k/N)} \approx \sum_{-\delta_l \le k/M \le \delta_u} w\left(\frac{k}{M}\right) e^{(2\pi ij/P)(k/N)},$$

with M a power of 2. This expression can be efficiently computed with the fractional FFT.

Remark 6.10: If the inversion point is close to a singularity, we can compute $f(t)$ accurately by inverting the scaled Laplace transform

$$f_{w_k}(t) = w_k(t) f(\Delta t).$$

To be more precise, suppose that f is smooth on the interval $[k - \delta_a, k + \delta_a]$ and that the function w_k has ϵ-support contained in $[k - \delta, k + \delta]$. If we choose $\Delta \le \delta_a/\delta$, then f_{w_k} is a smooth function. The price we have to pay for a small Δ is that the period of w_k is large and that we need a larger number of terms for an accurate approximation of the Fourier series (6.8).

We end this subsection with a discussion of the numerical results for eight test functions with singularities that were used in the overview article of Davies and Martin (cf. [12]). These results are presented in Table 5. The inversions are done in

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TABLE 5. Results for Continuous Nonanalytical Test Functions

No.	$\Delta = 1/16$	$\Delta = 1$	$\Delta = 10$
9	3e-14	2e-14	7e-15
10	4e-14	1e-14	4e-15
11	7e-15	2e-14	2e-14
12	5e-15	1e-15	6e-16
13	3e-16	9e-16	9e-17
14	1e-14	3e-15	8e-16
15	1e-14	2e-14	2e-14
16	1e-14	2e-14	2e-14

Note: The mean absolute error $\sum_{k=0}^{M-1} |e((k+1)\Delta)|/(1 + e((k+1)\Delta))$ is presented for the inversion of eight functions with singularities in $t = 0$ of Table 4. We have computed the function values in the points $\{1/16, 1/8 \ldots, 31/16\}$, $\{1,2,\ldots,31\}$, and $\{10,20,\ldots,310\}$. From this table, we can conclude that for functions with singularities the results are near machine accuracy.

32 points and so $M = 32$. We have taken $P = 256 = 8M$, and for all of the examples, we have taken $a = 44/M_2$. In addition to the choice of the previous parameters, we have taken $n = 48$, $\sigma = 6\sqrt{2}$, and $L = 6$. The computations are done with double precision. We have taken $\Delta = 1/16$, $\Delta = 1$, and $\Delta = 10$. We see that the approximation error seems to be independent of Δ. The reason for this is that the approximation error is dominated with round-off error and the error caused by the highly peaked window function. We also test the method on two discontinuous functions. These results are presented in Table 6. For this example, we have taken $\Delta = 1/16$. From all of the examples, we can conclude that the method is very accurate, robust, and fast.

TABLE 6. Results for Noncontinuous Test Functions

No.	Function	Laplace Transform	MAE
17	$H(t-1)$	$s^{-1}\exp(-s)$	1e-13
18	Square wave	$s^{-1}(1+\exp(-s))^{-1}$	1e-13

Note: The mean absolute error (MAE) is presented for the inversion of two noncontinuous functions in the points 0, $1/16 \ldots, 15/16, 17/16, \ldots, 31/16$. From this table, we can conclude that for noncontinuous functions, the results are also very accurate.

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APPENDIX A
Some Weights and Nodes for the Quadrature Rule

λ_j	β_j	λ_j	β_j
$n = 16$		$n = 48$	
4.44089209850063e-016	1	0	1
6.28318530717958	1.00000000000004	6.28318530717957	1
12.5663706962589	1.00000015116847	12.5663706143592	1
18.8502914166954	1.00081841700481	18.8495559215388	1
25.2872172156717	1.09580332705189	25.1327412287183	1
34.296971663526	2.00687652338724	31.4159265358979	1
56.1725527716607	5.94277512934943	37.6991118430775	1
170.533131190126	54.9537264520382	43.9822971502571	1
		50.2654824574367	1
$n = 32$		56.5486677646182	1.00000000000234
0	1	62.8318530747628	1.00000000319553
6.28318530717958	1	69.1150398188909	1.00000128757818
12.5663706143592	1	75.3984537709689	1.00016604436873
18.8495559215388	1	81.6938697567735	1.00682731991922
25.1327412287184	1	88.1889420301504	1.08409730759702
31.4159265359035	1.00000000000895	95.7546784637379	1.3631917322868
37.6991118820067	1.00000004815464	105.767553649199	1.85773538601497
43.9823334683971	1.00003440685547	119.58751936774	2.59022367414073
50.2716029125234	1.00420404867308	139.158762677521	3.73141804564276
56.7584358919044	1.09319461846681	168.156165377339	5.69232680539143
64.7269529917882	1.51528642466058	214.521886792255	9.54600616545647
76.7783110023797	2.4132076646714	298.972429369901	18.8912132110256
96.7780294888711	4.16688127092229	497.542914576338	52.7884611477405
133.997553190014	8.3777001312961	1494.71066227687	476.448331869636
222.527562038705	23.6054680083019		
669.650134867713	213.824023377988		

Note: λ_j and β_j for n = 16, 32, and 48.

We tabulated only the numbers λ_j and β_j for $j = 1,2,\ldots,n/2$. The numbers λ_{n+1-j} are given by $-\lambda_j - 2\pi$. The numbers β_{n+1-j} coincide with β_j.

APPENDIX B
The Fourier Transform

We start by introducing the Fourier transform over the space $L^1(-\infty,\infty)$ of Lebesgue integrable functions. For a function $f \in L^1(-\infty,\infty)$ and pure imaginary s, the Fourier integral

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$$\hat{f}(s) := \int_{-\infty}^{\infty} e^{-st} f(t)\, dt$$

is properly defined. In fact,

$$|\hat{f}(s)| \leq \int_{-\infty}^{\infty} |f(t)|\, dt = \|f\|_1 \tag{B.1}$$

and $\hat{f}$ is a continuous function. If the support of f is contained in $[0,\infty)$, then we call $\hat{f}$ the Laplace transform of f. If $\hat{f} \in L^1(-i\infty, i\infty)$, the space of complex-valued Lebesgue integrable functions, satisfies $(1/2\pi i)\int_{-i\infty}^{-i\infty} |f(s)|\, ds < \infty$, then the inverse Fourier integral is properly defined.

THEOREM B.1. *If $f \in L^1(-\infty,\infty)$ and $\hat{f} \in L^1(-i\infty, i\infty)$, then*

$$f(t) = \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} e^{st} \hat{f}(s)\, ds$$

is properly defined and

$$f(t) \leq \frac{1}{2\pi i} \int_{-i\infty}^{i\infty} |\hat{f}(s)|\, ds = \|\hat{f}\|_1.$$

This theorem can be found in any text about Fourier transforms; we have taken it from Mallat [15]. It follows immediately that $\hat{f} \in L^1(-i\infty, i\infty)$ iff f is a continuous function.

APPENDIX C
Gaussian Quadrature

DEFINITION C.1 (Gaussian Quadrature (cf. Szegő [24])): *Let the inner product $\langle \cdot,\cdot \rangle$ be given by*

$$\langle f, g \rangle = \int_I f(t) g^*(t) \mu(dt),$$

with μ a given positive measure and I a subinterval of the real axis or a subinterval of the imaginary axis. Let $\{q_k\}$ be an orthogonal set w.r.t. this inner product. Let the inner product $\langle \cdot,\cdot \rangle_n$ given by

$$\langle f, g \rangle_n := \sum_{k=1}^{n} \alpha_k f(\mu_k) g^*(\mu_k),$$

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with $\{\mu_k; k = 0,1,\ldots,n-1\}$ *the simple roots of* q_n *and the strictly positive numbers* $\{\alpha_k; k = 0,1,\ldots,n-1\}$, *the so-called Christophel numbers, be given by*

$$\alpha_k = \frac{1}{\sum_{j=1}^{n} |q_j(u_k)|^2} = \frac{A_n}{A_{n-1}} \frac{1}{\partial q_n(\mu_j)} \frac{1}{q_{n-1}^*(\mu_j)},$$

with A_n *the highest coefficient in* q_n. *The roots* $\{\mu_k; k = 0,1,\ldots,n-1\} \in I$. *The inner product* $\langle \cdot,\cdot \rangle_n$ *is called the Gaussian quadrature rule and is the unique nth-order quadrature rule satisfying*

$$\langle p, \mathbf{1} \rangle_n = \langle p, \mathbf{1} \rangle \quad \text{for all } p \in \pi_{2n-1},$$

where π_n *is the space of polynomials with degree not exceeding n and* **1** *is the constant function* $\mathbf{1}(t) = 1$.

APPENDIX D
Legendre Polynomials

The Legendre polynomials $\{\phi_n; n \in N_0\}$ are a complete orthogonal polynomial set in $L^2([0,1])$. These polynomials $\{\phi_n; n \in N_0\}$, $\phi_n: [0,1] \to \mathbb{R}$ are given by

$$\phi_n(t) = \frac{\sqrt{2n+1}}{n!} D^n(t^n(1-t)^n),$$

with D the differential operator.

Consider the polynomials

$$p_n(s) = \sqrt{2n+1} \sum_{k=0}^{n} \frac{(k+n)!}{(n-k)!} \frac{(-s)^k}{k!}.$$

A routine computation shows that the Laplace transform $\hat{\phi}_n$ of the nth Legendre polynomial ϕ_n is given by

$$\hat{\phi}_n(s) = \int_0^1 e^{-st}\phi_n(t)\,dt = \frac{1}{s}\left(p_n\left(\frac{1}{s}\right) - (-1)^n e^{-s} p_n\left(-\frac{1}{s}\right)\right).$$

Introduce

$$q_n^v(s) = (p_n(s) - (-1)^n e^{-2\pi i v} p_n(-s))$$

and $\Psi\hat{f}(s) = s^{-1}\hat{f}(s^{-1})$. Since $\exp(-s^{-1}) = \exp(-i2\pi v)$ on $\{(i2\pi(k+v))^{-1}, k \in \mathbb{Z}\}$, it follows that

$$q_n^v = \Psi\hat{\phi}_n \tag{D.1}$$

on $\{(i2\pi(k+v))^{-1}, k \in \mathbb{Z}\}$. This identity is crucial for Appendixes E and F.

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APPENDIX E
Proofs of Theorems 3.2 and 5.3

Proof of Theorem 3.2: Recall that

$$\hat{\phi}_n(s) = \frac{1}{s}\left(p_n\left(\frac{1}{s}\right) - (-1)^n e^{-s} p_n\left(-\frac{1}{s}\right)\right)$$

$$q_n^v(s) = (p_n(s) - (-1)^n e^{-2\pi i v} p_n(-s)),$$

and $\Psi \hat{f}(s) = s^{-1}\hat{f}(s^{-1})$. Since $\exp(-s^{-1}) = \exp(-i2\pi v)$ on $\{(i2\pi(k+v))^{-1}, k \in \mathbb{Z}\}$, it follows that $q_n^v = \Psi\hat{\phi}_n$, on $\{(i2\pi(k+v))^{-1}, k \in \mathbb{Z}\}$. Hence,

$$\langle q_m^v, q_n^v \rangle_{Q_v} = \langle \Psi\hat{\phi}_m, \Psi\hat{\phi}_n \rangle_{Q_v}.$$

Let

$$\Phi_{mn}(t) = \int_{-\infty}^{\infty} \phi_m(t-u)\phi_n(-u)\, du.$$

Since

$$\langle \Psi\hat{\phi}_m, \Psi\hat{\phi}_n \rangle_{Q_v} = \sum_{k=-\infty}^{\infty} \hat{\phi}_m(i2\pi(k+v))\hat{\phi}_n^*(i2\pi(k+v))$$

$$= \sum_{k=-\infty}^{\infty} \hat{\Phi}_{mn}(i2\pi(k+v))$$

and the function Φ_{mn} is of bounded variation and in L^1, we can apply the PSF (Theorem 2.1) and obtain that

$$\langle q_m^v, q_n^v \rangle_{Q_v} = \langle \Psi\hat{\phi}_m, \Psi\hat{\phi}_n \rangle_{Q_v} = \phi_{mn}(0) = \langle \phi_m, \phi_n \rangle.$$

This proves that the $\{q_j\}$ are orthogonal.

Define

$$Q_v \Psi \hat{f}(t) = \sum_{k=-\infty}^{\infty} \hat{f}(i2\pi(k+v))e^{-i2\pi(k+v)t}.$$

Since

$$\sum_{k=-\infty}^{\infty} |\hat{f}(i2\pi(k+v))|^2 < \infty,$$

range$(Q_v \Psi \hat{f}) \in L^2([0,1])$. Since $\{\phi_k\}$ is a complete orthogonal set in $L^2([0,1])$, we obtain that

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$$\sum_{k=-\infty}^{\infty} |\hat{f}(i2\pi(k+v))|^2 = \|Q_v \Psi \hat{f}\|^2 = \sum_{k=0}^{\infty} |\langle Q_v \Psi \hat{f}, \phi_k \rangle|^2.$$

Since

$$\langle e^{-2\pi i(v+j)\cdot}, \phi_k \rangle = \hat{\phi}_k(2\pi i(v+j)),$$

we obtain that

$$\sum_{k=0}^{\infty} |\langle Q_v \Psi \hat{f}, \phi_k \rangle|^2 = \sum_{k=0}^{\infty} |\langle \Psi \hat{f}, \Psi \hat{\phi}_k \rangle_{Q_v}|^2 = \sum_{k=0}^{\infty} |\langle \Psi \hat{f}, q_k^v \rangle_{Q_v}|^2;$$

in the last step, we use $q_n^v = \Psi \hat{\phi}_n$ on $\{(i2\pi(k+v))^{-1}, k \in \mathbb{Z}\}$. Thus,

$$\sum_{k=0}^{\infty} |\langle \Psi \hat{f}, q_k^v \rangle_{Q_v}|^2 = \sum_{k=-\infty}^{\infty} |\hat{f}(i2\pi(k+v))|^2.$$

We obtain from Parseval's theorem (cf. Conway [10, Thm. 4.13]) that $\{q_k^v\}$ is a complete orthogonal set in $L^2(Q_v)$. ■

Proof of Theorem 5.3: Since for $f(s,r) = f_1(s)f_2(r)$ and $g(s,r) = g_1(s)g_1(r)$,

$$\langle f, g \rangle_{Q_{v\omega}} = \langle f_1, g_1 \rangle_{Q_v} \langle f_2, g_2 \rangle_{Q_\omega},$$

the orthogonality of $\{q_{kj}^{v\omega}\}$ follows from the orthogonality of the sets $\{q_k^v\}$ and $\{q_j^v\}$ Let $\Psi \hat{f}(s,r)$ and $\Psi_s \hat{f}(s,r)$ denote $s^{-1}r^{-1}\hat{f}(s^{-1}, r^{-1})$ and $s^{-1}\hat{f}(s^{-1}, r)$, respectively. Since

$$\langle \Psi \hat{f}, q_{kj}^{v\omega} \rangle_{Q_{v\omega}} = \langle \langle \Psi \hat{f}, q_k^v \rangle_{Q_v}, q_j^\omega \rangle_{Q_\omega},$$

we obtain that

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} |\langle \Psi \hat{f}, q_{kj}^{v\omega} \rangle_{Q_{v\omega}}|^2 = \sum_{k=0}^{\infty} \sum_{j=0}^{\infty} |\langle \langle \Psi \hat{f}, q_k^v \rangle_{Q_v}, q_j^\omega \rangle_{Q_\omega}|^2.$$

Using the fact that the sets $\{q_k^v\}$ and $\{q_j^\omega\}$ are both complete orthogonal in $L^2(Q_v)$ and $L^2(Q_\omega)$, respectively, yields by Parseval's theorem (cf. Conway [10, Thm. 4.13]) that

$$\sum_{k=0}^{\infty} \sum_{j=0}^{\infty} |\langle \langle \Psi \hat{f}, q_k^v \rangle_{Q_v}, q_j^\omega \rangle_{Q_\omega}|^2 = \sum_{j=-\infty}^{\infty} \sum_{k=0}^{\infty} |\langle \Psi_s \hat{f}(\cdot, 2\pi i(j+\omega)), q_k^v \rangle_{Q_v}|^2$$

$$= \sum_{j=-\infty}^{\infty} \sum_{k=-\infty}^{\infty} |\hat{f}(2\pi i(k+v), 2\pi i(j+\omega))|^2.$$

We obtain from Parseval's theorem that $\{q_{kj}^{v\omega}\}$ is a complete orthogonal set in $L^2(Q_{v\omega})$. ■

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APPENDIX F
The Computation of $\{\mu_k^v\}$ and $\{\alpha_k^v\}$

Let us begin with analyzing the matrix representation of the multiplication operator w.r.t. the basis $\{q_k^v\}$.

THEOREM F.1: *Let $M: L^2_{Q_v} \to L^2_{Q_v}$ be the multiplication operator defined by $Mf(s) = sf(s)$. The matrix representation of M, $\hat{M}$, w.r.t. the basis $\{q_k^v\}$ is given by*

$$\begin{bmatrix} \frac{1}{2}\frac{1+\exp(-i2\pi v)}{1-\exp(-i2\pi v)} & -C_1 & & & \\ C_1 & 0 & -C_2 & & \\ & C_2 & 0 & \ddots & \\ & & \ddots & \ddots & \end{bmatrix},$$

where

$$C_n = \frac{1}{2}\frac{1}{\sqrt{4n^2-1}}.$$

Let $M_n: L^2_{Q_v^n} \to L^2_{Q_v^n}$ be the multiplication operator defined by $M_n f(s) = sf(s)$. The matrix representation of M_n, $\hat{M}_n$, w.r.t. the basis $\{q_k^v;\ k = 0,1,\ldots,n-1\}$ is given by

$$\begin{bmatrix} \frac{1}{2}\frac{1+\exp(-i2\pi v)}{1-\exp(-i2\pi v)} & -C_1 & & \\ C_1 & 0 & -C_2 & \\ & C_2 & \ddots & -C_{n-1} \\ & & C_{n-1} & 0 \end{bmatrix}.$$

PROOF: Since

$$\langle Mf, g\rangle_{Q_v} = \langle sf, g\rangle_{Q_v} = \langle f, s^* g\rangle_{Q_v} = -\langle f, Mg\rangle_{Q_v},$$

M is a skew adjoint operator. Since q_n is orthogonal to π_{n-1}, the space of polynomials with degree less or equal $n-1$, we obtain that

$$\langle Mq_j^v, q_k^v\rangle_{Q_v} = 0 \quad \text{for } j < k-1.$$

Since M is skew adjoint, we obtain that

$$\langle Mq_j^v, q_k^v\rangle_{Q_v} = 0 \quad \text{for } j > k+1.$$

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Let A_n be the coefficient of s^n in q_n^v and let B_n be the coefficient of s^{n-1} in q_n^v. It can be easily verified that

$$A_n = \sqrt{2n+1}\,\frac{(2n)!}{n!}(-1)^n(1-e^{-i2\pi v}),$$

$$B_n = \sqrt{2n+1}\,\frac{(2n-1)!}{(n-1)!}(-1)^{n-1}(1+e^{-i2\pi v}).$$

Comparing the coefficient of s^n in Mq_{n-1}^v and q_n^v respectively yields that

$$\langle Mq_{n-1}^v, q_n^v\rangle_{Q_v} = \frac{A_{n-1}}{A_n} = -\frac{1}{2}\frac{1}{\sqrt{4n^2-1}}.$$

Comparing the coefficients of s^n in $Mq_n^v - \langle Mq_n^v, q_{n+1}^v\rangle_{Q_v} q_{n+1}^v$ and q_n^v respectively yields that

$$\langle Mq_n^v, q_n^v\rangle_{Q_v} = \frac{B_n}{A_n} - \frac{B_{n+1}}{A_{n+1}} = 0, \qquad n \geq 1,$$

and

$$\langle Mq_0^v, q_0^v\rangle_{Q_v} = -\frac{B_{n+1}}{A_{n+1}} = \frac{1}{2}\frac{1+\exp(-i2\pi v)}{1-\exp(-i2\pi v)}.$$

Expanding Mq_n^v in $\{q_k^v\}$ yields the desired result for the operator M. Since for all $f \in L^2_{Q_v^n}$,

$$\langle f, q_{n+1}^v\rangle_{Q_v^n} = 0,$$

we obtain the desired result for the operator M_n. ■

THEOREM F.2: *The numbers $\{\mu_k^v\}$ are the eigenvalues of M_n. The Christophel numbers $\{\alpha_k^v\}$ are given by $|\langle v_k, q_0^v\rangle|^2/|1-\exp(-i2\pi v)|^2$, with the $\{v_k\}$ the normalized eigenfunctions $(\|v_k\| = 1)$ of M_n.*

PROOF: Let ρ be an arbitrary polynomial in π_{2n-1}. Since the matrix M_n is skew self-adjoint, we obtain by the spectral theorem (cf. Conway [10]) that

$$\langle \rho(M_n)\mathbf{1},\mathbf{1}\rangle_{Q_v^n} = \sum \rho(\lambda_k)|\langle \mathbf{1}, v_k\rangle_{Q_v^n}|^2 = \sum \rho(\lambda_k)\frac{|\langle v_k, q_0^v\rangle_{Q_v^n}|^2}{|1-\exp(-i2\pi v)|^2},$$

with $\{a_k\}$ the eigenvalues and $\{v_k\}$ the normalized eigenfunctions $(\|v_k\| = 1)$ of M_n. Further, since M_n and M are tridiagonal, we obtain that

$$\langle \rho\mathbf{1},\mathbf{1}\rangle_{Q_v^n}\frac{\langle \rho(\hat{M}_n)q_0^v, q_0^v\rangle_{Q_v^n}}{|1-\exp(-i2\pi v)|^2} = \frac{\langle \rho(M)q_0^v, q_0^v\rangle_{Q_v}}{|1-\exp(-i2\pi v)|^2} = \langle \rho\mathbf{1},\mathbf{1}\rangle_{Q_v}.$$

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Since the Gaussian quadrature rule is the unique nth-order quadrature rule satisfying

$$\langle p, \mathbf{1}\rangle_n = \langle p, \mathbf{1}\rangle \quad \text{for all } p \in \pi_{2n-1},$$

we obtain the result. ■

Remark F.3: Since the matrix $\hat{M}_n$ is skew self-adjoint, we can efficiently compute the eigenvalues $\{\mu_k^v\}$ and eigenvectors $\{v_k\}$ with the QR algorithm (cf. Stoer and Bulirsch [23]).

APPENDIX G
Error Analysis

Let us start by giving an alternative formula for the Christophel numbers $\{\alpha_j^v\}$.

LEMMA G.1: *The Christophel numbers $\{\alpha_j^v\}$ are given by*

$$\alpha_j^v = \left(\frac{A_n^v}{A_{n-1}^v}\right)^* \frac{1}{q_{n-1}^v(\mu_j^v)} \frac{-1}{Dq_{n-1}^{-v}(-\mu_k^v)},$$

where A_n^v is the coefficient of s^n in q_n^v.

PROOF: Let ℓ_j be the Lagrange polynomial defined by $\ell_j(\mu_k^v) = \delta_{kj}$, with $\delta_{kj} = 1$ if $k = j$ and $\delta_{kj} = 0$ if $k \neq j$. Then $\langle q_{n-1}^v, \ell_j\rangle = \alpha_j^v q_{n-1}^v(\mu_j^v)$. On the other hand, $\langle \ell_j, q_{n-1}^v\rangle = B_j/A_{n-1}^v$, with A_{n-1}^v the coefficient of s^{n-1} in q_{n-1}^v and B_j the coefficient of s^{n-1} in ℓ_j. Since $B_j = A_n^v/Dq_n^v(\mu_k^v)$, we obtain the identity

$$\alpha_j^v = \left(\frac{A_n^v}{A_{n-1}^v}\right)^* \frac{1}{q_{n-1}^v(\mu_j^v)} \frac{-1}{Dq_{n-1}^{-v}(-\mu_k^v)}.$$ ■

Before we can give an error estimate for the quadrature rule, we need the following technical lemma.

LEMMA G.2: *Let the integration operator $I: L^2([0,1]) \to L^2([0,1])$ be given by*

$$If(x) = \int_0^x f(t)\,dt.$$

For $m = 0,1,\ldots,n-1$, the estimate

$$\|s^m q_{n-1}^v\|_{Q_v^n} \leq \|I^m \phi_{n-1}\|$$

is valid.

PROOF: Since by the PSF (Theorem 2.1) $\|I^m\phi_{n-1}\| = \|s^m q_{n-1}^v\|_{Q_v}$ and $\|s^m q_{n-1}^v\|_{Q_v^n} = \|\hat{M}_n^m e_n\|$ and $\|s^m q_{n-1}^v\|_{Q_v} = \|\hat{M}^m e_n\|$, with e_n the nth unit vector, we only have to prove that $\|\hat{M}_n^m e_n\| \leq \|\hat{M}^m e_n\|$. Introduce the directed graph G with vertices $\{0,1,\ldots\}$ and edges $V^- = \{V_{j,j+1}\}$ and $V^+ = \{V_{j,j-1}\}$. Let G_n be the subgraph of G with vertices $\{0,1,\ldots,n-1\}$ and edges $V^- = \{V_{j,j+1};\ j \leq n-2\}$ and $V^+ = \{V_{j,j-1};\ j \leq n-1\}$. Let the weight of the path $\{j_0,\ldots,j_m\}$ be

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given by $\prod_{p=0}^{m-1} M_{j_p j_{p+1}}$. Let S_k^m and $\hat{S}_k^m$ be the set of all paths from $n-1$ to k of length m in G and G_n, respectively. The remainder of the proof consists of the following steps:

(1) $\langle M^m e_n, e_k\rangle = \sum_{x\in S_k^m} \prod_{p=1}^m M_{x_p x_{p+1}}$ and $\langle M_n^m e_n, e_k\rangle = \sum_{x\in \hat{S}_k^m} \prod_{p=1}^m M_{x_p x_{p+1}}$.
(2) The weight of each path in S_k^m has the same sign.
(3) $|\langle M_n^m e_n, e_k\rangle| \le |\langle M^m e_n, e_k\rangle|$ and $\|M_n^m e_n\| \le \|M_n^m e_n\|$.

Proof of Step (1): We will prove this result by induction. Clearly, the result is true for $m = 1$. Since

$$S_k^{m+1} = \{S_{k-1}^m, (k-1,k)\} \cup \{S_{k+1}^m, (k+1,k)\},$$

we obtain

$$\begin{aligned}\sum_{j\in S_{m+1}^k} \prod_{p=1}^{m+1} \hat{M}_{j_p j_{p+1}} &= \hat{M}_{k-1k} \sum_{j\in S_m^{k-1}} \prod_{p=1}^{m} \hat{M}_{j_p j_{p+1}} + \hat{M}_{k+1k} \sum_{j\in S_m^{k+1}} \prod_{p=1}^{m} \hat{M}_{j_p j_{p+1}}\\ &= \hat{M}_{k-1k}\langle \hat{M}^m e_n, e_{k-1}\rangle + \hat{M}_{k+1k}\langle \hat{M}^m e_n, e_{k+1}\rangle\\ &= \langle \hat{M}^{m+1} e_n, e_k\rangle,\end{aligned}$$

where the second equation follows from the induction hypotheses and the last equality follows from the fact that the matrix $\hat{M}$ is tridiagonal (Theorem F.1) with only the first element on the diagonal nonzero and $m \le n-1$.

Proof of Step (2): Since each path from $n-1$ to k contains exactly $(m-(n-1-k))/2$ edges of the set V^- and $(m+(n-1-k))/2$ edges of the set V^+, the weight of each path in S_k^m has the same sign.

Proof of Step (3): Since $\hat{S}_k^m$ is a subset of S_k^m and each path in S_k^m has the same sign, we obtain

$$|\langle \hat{M}_n^m e_n, e_k\rangle| = \sum_{x\in \hat{S}_k^m} \left| \prod_{p=1}^m \hat{M}_{x_p x_{p+1}} \right| \le \sum_{x\in S_k^m} \left| \prod_{p=1}^m \hat{M}_{x_p x_{p+1}} \right| = |\langle \hat{M}^m e_n, e_k\rangle|.$$

The desired result follows from

$$\|\hat{M}_n^m e_n\|^2 = \sum_{k=0}^{n-1} |\langle \hat{M}_n^m e_n, e_k\rangle|^2 \le \sum_{k=0}^{n-1} |\langle \hat{M}^m e_n, e_k\rangle|^2 \le \|\hat{M}^m e_n\|^2. \qquad \blacksquare$$

We can now give an error estimate for the quadrature rule.

THEOREM G.3: *The error of the quadrature formula*

$$E_v \hat{f} = \langle \Psi\hat{f}, \Psi\mathbf{1}\rangle_{Q_v} - \langle \Psi\hat{f}, \Psi\mathbf{1}\rangle_{Q_v^n}$$

is given by

$$\frac{1}{2}\,\frac{(-1)^n}{\sqrt{4n^2-1}} \sum_{j=1}^{\infty} j e^{-i2\pi j v} W_{j-1} f^{(2)} + \xi\hat{f},$$

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where $f^{(k)}$ denotes the kth-order derivative of f and

$$W_j h = \int_0^1 \int_0^1 h(j+t+y)\phi_n(t)\phi_{n-1}(y)\,dy\,dt,$$

with ϕ_n the nth Legendre polynomials given by

$$\phi_n(t) = \frac{\sqrt{2n+1}}{n!} D^n(t^n(1-t)^n),$$

where D denotes the differential operator. Furthermore, the remainder $\xi\hat{f}$ is bounded by

$$|\xi\hat{f}| \le \frac{1}{4} \min_{0\le m\le(n-1)} \frac{\|I^m\phi_{n-1}\|^2}{4n^2-1} \sum_{j=0}^{\infty} (j+1)\|R_j f^{(4+2m)}\|_1,$$

with

$$R_j h(x) = \begin{cases} 0, & x<0 \\ \int_0^1\int_0^1 h(j+t+y+x)\phi_n(t)\phi_n(y)\,dy\,dt, & x\ge 0. \end{cases}$$

Moreover,

$$W_j h = \sqrt{4n^2-1}\,\frac{(n-1)!}{(2n-1)!}\,\frac{n!}{(2n+1)!}\,h^{(2n-1)}(\alpha_j), \qquad \alpha_j \in (j, j+2),$$

$$\|R_j h\|_1 \le (2n+1)\left(\frac{n!}{(2n+1)!}\right)^2 \|h_j^{(2n)}\|_1,$$

$$\|I^{n-1}\phi_{n-1}\|^2 = \frac{(2n-1)}{(n-1!)^2}\left(\frac{((2n-2)!)^2}{(4n-3)!}\right),$$

where

$$\|h_j^{(2n)}\|_1 = \int_j^\infty |h_j^{(2n)}(t)|\,dt.$$

Thus, for smooth functions,

$$E_v\hat{f} \approx \frac{1}{2}(-1)^n \frac{(n-1)!n!}{(2n-1)!} \sum_{j=1}^{\infty} je^{-i2\pi jv} \frac{f^{(2n+1)}(j-1+\alpha)}{(2n+1)!},$$

with α some number in $(0,2)$.

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PROOF: The proof consists of the following steps:

(1) The functional E_v can be expanded as

$$E_v \hat{f} = -\frac{1}{2}\frac{1}{\sqrt{4n^2-1}}\sum_{j=0}^{\infty} e^{-i2\pi jv}\langle q_{n-1}^v \Psi \widehat{V_j Df}, \Psi \mathbf{1}\rangle_{Q_v^n}, \quad \textbf{(G.1)}$$

where V_j is given by

$$V_j h(y) = \begin{cases} 0, & y < 0 \\ \int_0^1 h(j+t+y)\phi_n(t)\,dt, & y \geq 0. \end{cases}$$

(2) By the definition of the functional E_v,

$$E_v(q_{n-1}^v(s^{-1})\widehat{V_j Df}) = \langle q_{n-1}^v \Psi \widehat{V_j f}, \Psi \mathbf{1}\rangle_{Q_v} - \langle q_{n-1}^v \Psi \widehat{V_j f}, \Psi \mathbf{1}\rangle_{Q_v^n}. \quad \textbf{(G.2)}$$

The term $\langle q_{n-1}^v \Psi \widehat{V_j f}, \Psi \mathbf{1}\rangle_{Q_v}$ is equal to

$$(-1)^{n-1}\sum_{k=0}^{\infty} e^{-i2\pi(k+1)v}\int_0^1\int_0^1 f^{(2)}(k+j+t+u)\phi_n(t)\phi_{n-1}(y)\,dy\,dt. \quad \textbf{(G.3)}$$

(3) The term $|\langle q_{n-1}^v q_{n-1}^v \Psi \widehat{R_{j+k} D^2 f}, \Psi \mathbf{1}\rangle_{Q_v^n}|$ is bounded by

$$\|I^m \phi_{n-1}\|\,\|R_{j+k} f^{4+2m}\|_1.$$

(4) We can estimate $W_j h$ and $\|R_j h\|_1$ by

$$W_j h = \sqrt{(2n)^2-1}\,\frac{(n-1)!}{(2n-1)!}\,\frac{n!}{(2n+1)!}\,h^{(2n-1)}(\alpha), \qquad \alpha \in (j, j+2),$$

$$\|R_j h\|_1 \leq (2n+1)\left(\frac{n!}{(2n+1)!}\right)^2 \|h_j^{(2n)}\|_1.$$

Proof of Step (1): Let $\hat{g}(s) = s\hat{f}(s)$; then

$$\langle \Psi \hat{f}, \Psi \mathbf{1}\rangle_{Q_v} = -\langle \Psi \hat{g}, \mathbf{1}\rangle_{Q_v} \quad \text{and} \quad \langle \Psi \hat{f}, \Psi \mathbf{1}\rangle_{Q_v^n} = -\langle \Psi \hat{g}, \mathbf{1}\rangle_{Q_v^n}.$$

Let P_{n-1} be the interpolation polynomial of $\Psi \hat{g}$ in $\{\mu_k^v\}$, where the $\{\mu_k^v\}$ are the zeros of q_n^v. Since the quadrature rule is exact for polynomials of degree $n-1$, we obtain that

$$\langle P_{n-1}, \mathbf{1}\rangle_{Q_v} = \langle P_{n-1}, \mathbf{1}\rangle_{Q_v^n} = \langle \Psi \hat{g}, \mathbf{1}\rangle_{Q_v^n}.$$

Hence,

$$E_v \hat{f} = \langle \Psi \hat{g}, \mathbf{1}\rangle_{Q_v^n} - \langle \Psi \hat{g}, \mathbf{1}\rangle_{Q_v} = -\langle \Psi \hat{h}, \mathbf{1}\rangle_{Q_v},$$

with

$$\hat{h}(s) = \hat{g}(s) - \Psi P_{n-1}(s).$$

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Since for $s \in \{2\pi i(k+v)\}$ (cf. (D.1))

$$\frac{-s\hat{\phi}_n(-s)}{q_n^{-v}(-s^{-1})} = 1,$$

we obtain

$$-\langle \Psi\hat{h}, \mathbf{1}\rangle_{Q_v} = \langle \Psi\hat{k}, \Psi\mathbf{1}\rangle_{Q_v}, \tag{G.4}$$

with

$$\hat{k}(s) = s\hat{h}(s)\hat{\phi}_n(-s)\hat{W}(s),$$

where

$$\hat{W}(s) = -\frac{1}{s}\frac{1}{q_n^{-v}(-s^{-1})}.$$

The following observations show that $\hat{k}$ is a proper Laplace transform, satisfying the conditions for the PSF (Theorem 2.1):

(1) Since P_{n-1} interpolates $\Psi\hat{g}$ in $\{\mu_k^v\}$, the function $\hat{k}$ is holomorphic in $\{1/\mu_k^v\}$.
(2) Since $\hat{\phi}_n(-s) = O(s^n)$ and $1/q_n^{-v}(-s^{-1}) = O(s^n)$ in a neighborhood of zero, $\hat{k}$ is holomorphic in a neighborhood of zero.
(3)

$$\frac{\hat{k}(s)}{\hat{f}(s)} \to \frac{1-(-1)^n e^s}{1-(-1)^n e^{i2\pi v}} \quad \text{as } s \to \pm i\infty.$$

(4) $\hat{k}$ is holomorphic in the right half-plane $\Pi = \{s; \operatorname{Re}(s) > 0\}$. Thus,

$$\langle \Psi\hat{k}, \Psi\mathbf{1}\rangle_{Q_v} = \sum_{j=0}^{\infty} e^{-i2j\pi v} k(j),$$

with

$$k(x) = \frac{1}{2\pi i}\int_{-a-i\infty}^{-a+i\infty} e^{sx}\hat{k}(s)\,ds, \qquad a > 0.$$

Since $\hat{W}$ is holomorphic in the plane except in the points $\{1/\mu_k^v\}$ and converges uniformly to zero as $|s| \to \infty$, we obtain

$$W(x) = \begin{cases} 0 & \text{for } x \geq 0 \\ \displaystyle\sum_{k=1}^{n} \operatorname{res}\left(e^{sx}\hat{W}(s); s = \frac{1}{\mu_k^v}\right) & \text{for } x < 0. \end{cases}$$

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Hence, we obtain for $x < 0$,

$$W(x) = -\sum_{j=1}^{n} \frac{e^{x/\mu_j^v}}{\mu_j^v} \frac{1}{Dq_n^{-v}(-\mu_j^v)} \tag{G.5}$$

$$= -\frac{1}{2}\frac{1}{\sqrt{4n^2-1}} \sum_{j=1}^{n} \alpha_j^v \frac{e^{x/\mu_j^v}}{\mu_j^v} q_{n-1}^v(\mu_j^v),$$

where the last equality follows from Lemma G.1. Since the support of W is $(-\infty,0]$, we obtain

$$k(x) = \int_0^\infty \int_0^1 h^{(1)}(x+t+y)\phi_n(t)\,dtW(-y)\,dy,$$

$$= \int_0^\infty \int_0^1 f^{(2)}(x+t+y)\phi_n(t)\,dtW(-y)\,dy;$$

in the last equality we use that ϕ_n is orthogonal on each polynomial of degree less than n. By (G.5) and the definition of the inner product $\langle \cdot,\cdot \rangle_{Q_v^n}$ (Definition 3.3), this yields

$$k(j) = -\frac{1}{2}\frac{1}{\sqrt{4n^2-1}} \langle q_{n-1}^v \Psi \widehat{V_j f}^{(2)}, \Psi \mathbf{1} \rangle_{Q_v^n},$$

with V_j given by

$$V_j h(y) = \begin{cases} 0, & y < 0 \\ \displaystyle\int_0^1 h(j+t+y)\phi_n(t)\,dt, & y \geq 0. \end{cases}$$

Proof of Step (2): Since for $s \in \{2\pi i(k+v)\}$,

$$q_{n-1}^v(s^{-1}) = (-1)^{n-1} s e^{-i2\pi v} \hat{\phi}_{n-1}(-s),$$

the first term of (G.2) is equal to

$$(-1)^{n-1} e^{-i2\pi v} \langle \Psi(\hat{\phi}_{n-1}(-s)\widehat{V_j f}^{(2)}), \Psi \mathbf{1} \rangle_{Q_v}.$$

We obtain from the PSF (Theorem 2.1) that this is equal to

$$(-1)^{n-1} \sum_{k=0}^{\infty} e^{-i2\pi(k+1)v} \int_0^1 \int_0^1 f^{(2)}(k+j+t+u)\phi_n(t)\phi_{n-1}(y)\,dy\,dt. \tag{G.6}$$

We obtain from (G.1) that the second term of (G.2) is equal to

$$\frac{1}{2}\frac{1}{\sqrt{4n^2-1}} \sum_{k=0}^{\infty} e^{-i2\pi k v} \langle q_{n-1}^v q_{n-1}^v \Psi \widehat{R_{j+k} f}^{(2)}, \Psi \mathbf{1} \rangle_{Q_v^n},$$

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with

$$R_j h(x) = \begin{cases} 0, & x < 0 \\ \int_0^1 \int_0^1 h(j+t+y+x)\phi_n(t)\phi_n(y)\,dy\,dt, & x \geq 0. \end{cases}$$

Proof of Step (3): Since ϕ_n is orthogonal on π_{n-1}, we obtain $R_j p_{2n-1} = 0$ for $p_{2n-1} \in \pi_{2n-1}$. Hence,

$$\langle q_{n-1}^v q_{n-1}^v \widehat{\Psi R_{j+k} D^2 f}, \Psi \mathbf{1}\rangle_{Q_v^n} = (-1)^{n-1} e^{-i2\pi v} \widehat{\langle R_{j+k} f}^{(4+2m)} s^{2m} q_{n-1}^v, q_{n-1}^v\rangle_{Q_v^n}$$

for $0 \leq m \leq (n-1)$. Hence,

$$\begin{aligned} |\langle q_{n-1}^v q_{n-1}^v \widehat{\Psi R_{j+k} f^{(2)}}, \Psi \mathbf{1}\rangle_{Q_v^n}| &\leq \sup_s |\widehat{R_{j+k} f}^{(4+2m)}(s)|\,|\langle s^{2m} q_{n-1}^v, q_{n-1}^v\rangle_{Q_v^n}| \\ &\leq \|R_{j+k} f^{(4+2m)}\|_1 |\langle s^{2m} q_{n-1}^v, q_{n-1}^v\rangle_{Q_v^n}|, \end{aligned} \tag{G.7}$$

the last inequality follows from (A.1). We obtain from Lemma G.2 that

$$|\langle s^{2m} q_{n-1}^v, q_{n-1}^v\rangle_{Q_v^n}| = \|I^m \phi_{n-1}\|^2.$$

Proof of Step (4): Recall that

$$\phi_n(t) = \frac{\sqrt{2n+1}}{n!} D^n(t^n(1-t)^n).$$

Integration by part and using

$$D^{n-k}(t^n(1-t)^n)|_{t=0}^1 = 0, \qquad k = 1, \ldots, n,$$

yields that

$$\begin{aligned} W_j h &= \int_0^1 \int_0^1 h(j+t+y)\phi_n(t)\phi_{n-1}(y)\,dy\,dt \\ &= \sqrt{(2n)^2-1}\,\frac{(n-1)!}{(2n-1)!}\,\frac{n!}{(2n+1)!} \int_0^1 \int_0^1 h^{(2n-1)}(j+t+y) B_n(t) B_{n-1}(y)\,dy\,dt, \end{aligned}$$

where B_n is the density of the Beta distribution; that is,

$$B_n(t) = \frac{(2n+1)!}{n!n!} t^n(1-t)^n.$$

Since the Beta distribution is a probability distribution, we obtain by the mean value theorem that

$$W_j h = \sqrt{(2n)^2-1}\,\frac{(n-1)!}{(2n-1)!}\,\frac{n!}{(2n+1)!} D^{2n-1} h(\alpha_j), \qquad \alpha_j \in (j, j+2).$$

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Similarly,

$$R_j h(x) = \int_0^1 \int_0^1 h(j+t+y)\phi_n(t)\phi_n(y)\,dy\,dt$$
$$= (2n+1)\left(\frac{n!}{(2n+1)!}\right)^2 \int_0^1 \int_0^1 D^{2n}h(j+x+t+y)B_n(t)B_n(y)\,dy\,dt.$$

Hence,

$$\|R_j h\|_1 \le (2n+1)\left(\frac{n!}{(2n+1)!}\right)^2 \|D^{2n}h_j\|_1.$$

By a similar argument, we obtain

$$\|I^{n-1}\phi_{n-1}\|^2 = \frac{(2n-1)}{(n-1!)^2}\left(\frac{((2n-2)!)^2}{(4n-3)!}\right). \qquad ■$$

Remark G.4: It follows from Theorem G.3 that the approximation error does not depend on the discontinuity of f in $t = 0$.

APPENDIX H
On the Inversion of the *z*-Transforms

THEOREM H.1: *Let*

$$F(v) = \sum_{k=-\infty}^{\infty} f_k \exp(-2\pi i k v).$$

The following inversion formula holds:

$$\frac{1}{N}\sum_{k=0}^{N-1} F\left(\frac{k}{N}\right)\exp\left(2\pi i j\frac{k}{N}\right) = \sum_{m=-\infty}^{\infty} f_{mN+j}, \qquad \textbf{(H.1)}$$

for $j = 0, 1, \ldots, N-1$.

PROOF: Since for integral k and m, $\exp(-i2\pi km) = 1$, we obtain that

$$F\left(\frac{k}{N}\right) = \sum_{j=0}^{N-1}\sum_{m=-\infty}^{\infty} f_{mN+j}\exp\left(-2\pi i j\frac{k}{N}\right)\exp(-2\pi i k m)$$
$$= \sum_{j=0}^{N-1}\exp\left(-2\pi i j\frac{k}{N}\right)\sum_{m=-\infty}^{\infty} f_{mN+j}.$$

Hence,

$$\frac{1}{N}\sum_{k=0}^{N-1} F\left(\frac{k}{N}\right)\exp\left(2\pi i j\frac{k}{N}\right) = \frac{1}{N}\sum_{k=0}^{N-1} F_N\left(\frac{k}{N}\right)\exp\left(2\pi i j\frac{k}{N}\right),$$

with

$$F_N(v) = \sum_{j=0}^{N-1}\exp(-2\pi i j v)\sum_{m=-\infty}^{\infty} f_{mN+j}.$$

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Formula (H.1) follows from

$$\frac{1}{N}\sum_{k=0}^{N-1} F_N\left(\frac{k}{N}\right)\exp\left(2\pi ij\frac{k}{N}\right) = \sum_{m=-\infty}^{\infty} f_{mN+j}. \qquad \blacksquare$$

Remark H.2: This result is sometimes called the discrete Poisson summation formula (cf. Abate and Whitt [3]). In their article Abate and Whitt presented an efficient inversion algorithm for the inversion of z-transforms (also called generating functions) of discrete probability distributions.

We proceed as the article by Abate and Whitt [3]. It follows immediately from Theorem H.1 that if the discretization error

$$\xi_j := \sum_{m\neq 0,\, m\in\mathbb{Z}} f_{mN+j}$$

is small, then

$$f_j \approx \frac{1}{N}\sum_{k=0}^{N-1} F\left(\frac{k}{N}\right)\exp\left(2\pi ij\frac{k}{N}\right).$$

In general, it is hard to ensure that the discretization error ξ_d is small. However, for a special class of z-transforms, we can easily control the discretization error ξ_d. A z-transform, $\hat{f}$ belongs to the Hilbert space $H^2(\mathbb{U})$ if $\hat{f} \in L^2(\mathbb{T})$ and $f_k = 0$, for $k < 0$ (cf. Rudin [20, Chap. 17]). Since $f_k = 0$, for $k < 0$, we obtain that the inverse sequence of the z-transform $\widehat{f^r}(z) = \hat{f}(rz)$ is given by $\{r^k f_k; k \in \mathbb{N}\}$. Hence, $r^{-k} f_k^r = f_k$ and

$$\begin{aligned}\xi_j^r &:= r^{-j}\sum_{m=1}^{\infty} f_{mN+j}^r \\ &= \sum_{m=1}^{\infty} r^{mN} f_{mN+j}^r\end{aligned}$$

is of order $O(r^N)$. Hence, we can make ξ_j^r arbitrarily small by choosing r small enough. The conclusion is that if $\hat{f} \in H^2(\mathbb{U})$, then we can efficiently compute the numbers f_k with arbitrary precision, with the following algorithm.

Step 1. Set $\widehat{f^r}(z_k) = \hat{f}(rz_k)$, $k = 0,1,\ldots,m_2$.

Step 2. Compute $\widehat{f^r}(z_k) \to f_r$ with the m_2 points FFT algorithm and set $f_k = r^{-k} f_k^r$, $k = 0,1,\ldots,m$.

Remark H.3: On one hand, we want to choose r as small as possible, since then the discretization error is as small as possible. On the other hand, we multiply f_k^r by the factor r^{-k}; hence, a small r makes the algorithm numerically unstable. Suppose that we want to compute the values $\{f_k; k = 0,1,\ldots,m-1\}$ with a precision of ϵ. We can control both the discretization error and the numerical stability by using an $m_2 = 2^p m$ (with p a positive integral number) discrete Fourier transform (FFT) and choose $r = \epsilon^{1/m_2}$. The discretization error is then of magnitude ϵ and the multiplication factor is bounded by $\epsilon^{1/2^p}$. For double precision, we recommend the parameter values $p = 3$ and $r = \exp(-44/2^p m)$.

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