Operations Research Letters 12 (1992) 245–251
North-Holland

October 1992

Numerical inversion of probability generating functions

Joseph Abate
900 Hammond Road, Ridgewood, NJ 07450-2908, USA

Ward Whitt
AT & T Bell Laboratories, Room 2C-178, Murray Hill, NJ 07974-0636, USA

Received July 1991
Revised May 1992

Random quantities of interest in operations research models can often be determined conveniently in the form of transforms. Hence, numerical transform inversion can be an effective way to obtain desired numerical values of cumulative distribution functions, probability density functions and probability mass functions. However, numerical transform inversion has not been widely used. This lack of use seems to be due, at least in part, to good simple numerical inversion algorithms not being well known. To help remedy this situation, in this paper we present a version of the Fourier-series method for numerically inverting probability generating functions. We obtain a simple algorithm with a convenient error bound from the discrete Poisson summation formula. The same general approach applies to other transforms.

numerical inversion of transforms; computational probability; generating functions; Fourier-series method; Poisson summation formula; discrete Fourier transform

1. Introduction and summary

The analysis of stochastic models in operations research increasingly involves algorithms for computing probability distributions of interest. There are many useful tools for this purpose, but one that does not seem to be sufficiently well appreciated is numerical transform inversion.

Numerical transform inversion is especially attractive for queueing models, because many probability distributions of interest can be (or have been) characterized in the form of transforms. However, queueing textbooks provide remarkably little guidance. Indeed, there currently seems to be a trend to avoid transforms altogether. While alternative techniques are often effective, we contend that it is often surprisingly easy to extract useful numerical results from transforms.

To make a case for numerical transform inversion, in this paper we present and explain a simple algorithm for numerically inverting probability generating functions based on the Fourier-series method. Variants of the same method apply to other transforms, as can be seen from our longer review in [1]. We relate our algorithm to the literature in Remark 1 below; see [1] for further discussion.

The Fourier-series method can be interpreted as numerically integrating a standard inversion integral by means of the trapezoidal rule (which turns out to be surprisingly effective). The same formula is obtained by using the Fourier series of an associated periodic function constructed by aliasing. (For the sequences considered here, the discrete Fourier transform plays the role of the Fourier series.) The key mathematical result is the Poisson summation formula, which identifies the discretization error associated with the trapezoidal rule and thus helps bound it. For characteristic functions and Laplace

Correspondence to: Ward Whitt, AT&T Bell Laboratories, Room 2C-178, Murray Hill, NJ 07974-0636, USA.

0167-6377/92/$05.00

transforms of real-valued functions of a real variable, the inversion integral is over an unbounded interval, so that the approximating sum also needs to be truncated, which is the most difficult step. However, for generating functions, the inversion integral is over a finite interval, so that no truncation is needed. Thus, for most problems involving probability generating functions we obtain a simple computation with a guaranteed error bound.

Suppose that we wish to calculate terms from a sequence of real numbers $\{q_k: q \geqslant 0\}$ with $|q_k| \leqslant 1$ for all k using the generating function (or z-transform)

$$G(z) = \sum_{k=0}^{\infty} q_k z^k, \tag{1}$$

where z is a complex number. In particular, we assume that $G(z)$ can be evaluated for any given z, and our object is to obtain an approximation (with predetermined error bound) for q_k as a function of $G(z_1), \ldots, G(z_n)$ for finitely many complex numbers $z_1, \ldots, z_n$. The bound $|q_k| \leqslant 1$ automatically holds when q_k is a probability. Hence, in the applications we have in mind, there is nothing extra to verify. This known bound plays an important role in the error analysis, but it is not absolutely essential. Since $|q_k| \leqslant 1$, $G(z)$ is finite and analytic for all $|z| < 1$. The following theorem provides a simple algorithm with an error bound. (We prove the theorem in Section 2.) Let $\mathrm{i} = \sqrt{-1}$ and let $\mathrm{Re}(z)$ be the real part of z.

Theorem 1. *For* $0 < r < 1$ *and* $k \geqslant 1$.

$$|q_k - \tilde{q}_k| \leqslant \frac{r^{2k}}{1 - r^{2k}}.$$

where

$$\tilde{q}_k = \frac{1}{2kr^k} \sum_{j=1}^{2k} (-1)^j \, \mathrm{Re}\big(G(r\, \mathrm{e}^{\pi j \mathrm{i}/k})\big)$$

$$= \frac{1}{2kr^k} \left\{ G(r) + (-1)^k G(-r) + 2 \sum_{j=1}^{k-1} (-1)^j \, \mathrm{Re}\big(G(r\, \mathrm{e}^{\pi j \mathrm{i}/k})\big) \right\}.$$

We call the algorithm based on Theorem 1 LATTICE-POISSON (because it is for lattice distributions and because of the central role played by the Poisson summation formula). To show how easy LATTICE-POISSON is to perform, we display below a UBASIC program to calculate the complementary cdf of the number of customers served in an M/M/1 busy period. UBASIC is a public-domain high-precision version of BASIC created by Kida [9] to do mathematics on a personal computer; see Neumann [11]. UBASIC permits complex numbers to be specified conveniently and it represents numbers and performs computations with up to 100-decimal-place accuracy. (Diskettes containing UBASIC and the algorithm LATTICE-POISSON are available from the authors. An electronic file containing a C++ program is also available from the authors.) However, ordinary BASIC, FORTRAN or C with double precision would suffice. We discuss the particular M/M/1 example further in Section 3.

The UBASIC program

```
1 'The Algorithm LATTICE-POISSON
2 '
3 'A variant of the Fourier-series method
4 'for lattice distributions
5 'applied to the complementary cdf of the number of customers
6 'served in an M/M/1 busy period
7 '
20 input "LATTICE POINT =";N
21 E=8
```

```
22 R =1 / 10^(E / (2*N))
23 H =#pi / N
24 U =1 / (2*N*R^N)
25 '
30 Sum =0
31    for K =1 to N -1
32    Z =R*exp(#i*H*K)
33    Sum + =((-1)^K)*fnGen(Z):next
34 Sum =2*Sum +fnGen(R) +(-1)^N*fnGen(-R)
35 Fun =U*Sum
36 '
40 print
41 print "LATTICE POINT =";N,"FUNCTION =";using(2,7),Fun
42 end
43 '
80 fnGen(Z)
81 Rho =0.75:Bt =4*Rho / (1 +Rho)^2
82 Gz =(1 -sqrt(1 -Bt*Z)) / sqrt(Bt*Rho)
83 Gnz =(1 -Gz) / (1 -Z)
84 return(re(Gnz))
```

Remarks 1. We do not regard Theorem 1 as new, but it does not seem to be very well known. Indeed, the methods supporting Theorem 1 are classical, but we know of no explicit statement. The essential idea is expressed in Section 1 of Lyness [10], but the focus there is on further analysis using the Möbius function to treat the case in which we need *not* have $|q_k| \leqslant 1$ for all k. Essentially the same algorithm was proposed without error analysis by Cavers [3]. Nearly equivalent algorithms were also proposed by Jagerman [7,8] and Hosono [6]. Daigle [4] draws on the same ideas, but his algorithm is more complicated since he considers the special case with $r = 1$.

2. The algorithm LATTICE-POISSON is by no means the only way to calculate q_k from (1). Procedures for numerically differentiating (1) are incorporating in mathematical software packages such as MACSYMA, MATHEMATICA and MAPLE. For example, the M/M/1 busy-period probabilities in Section 3 are also easily calculated this way.

3. For practical purposes, we think of the error bound in Theorem 1 as r^{2k}, because $r^{2k}/(1-r^{2k})$ is approximately equal to r^{2k} when r^{2k} is small. Hence, to have accuracy to $10^{-\gamma}$, we let $r = 10^{-\gamma/2k}$. In the displayed program, we set $\gamma = E = 8$ on line 21 and set r in this manner on line 22.

4. We are primarily interested in probability applications for which $|q_k| \leqslant 1$ for all k. If $\{q_k\}$ does not initially have this property, then we may be able to work with $q'_k = aq_k b^k$ with generating function $G'(z) = aG(bz)$.

5. Of course, the finite sum in Theorem 1 is not easy to compute if k is extremely large, but for most operations research applications the indices k of interest are not extremely large. Moreover, for very large k, we would suggest using asymptotic analysis. This is illustrated for the example in Section 3.

6. Even for small k, computing the finite sum in Theorem 1 involves a potential roundoff error problem. The potential roundoff is evident from the multiplication by r^{-k}, which by Remark 2 is $10^{\gamma/2}$ when $10^{-\gamma}$ accuracy is desired. Assuming that $q_k \geqslant 0$ for all k, the terms in the finite sum are all bounded by $G(1) = \Sigma_{k=0}^{\infty} q_k$. Thus, if $G(1)$ is of order 1, then approximately $3\gamma/2$-digit precision is needed to obtain $10^{-\gamma}$ accuracy. For further discussion, see Remark 5.8 of [1].

2. Derivation and discussion of Theorem 1

Given the generating function $G(z)$ in (1), we can express the terms of the sequence $\{q_k\}$ via a Cauchy contour integral as

$$q_k = \frac{1}{2\pi \mathrm{i}} \int_{C_r} \frac{G(z)}{z^{k+1}} \, \mathrm{d}z, \tag{2}$$

where C_r is a circle about the origin of radius r, $0 < r < 1$. Upon making the change of variables $z = re^{iu}$, we obtain the expression

$$q_k = \frac{1}{2\pi r^k} \int_0^{2\pi} G(r\,e^{iu})\,e^{-iku}\,du$$
$$= \frac{1}{2\pi r^k} \int_0^{2\pi} \left[\cos ku\,\mathrm{Re}(G(r\,e^{iu})) + \sin ku\,\mathrm{Im}(G(r\,e^{iu}))\right] du, \tag{3}$$

where $\mathrm{Im}(z)$ is the imaginary part of z. If we calculate (3) approximately using the trapezoidal rule with a step size of π/k, then we obtain

$$q_k \approx \frac{1}{2\pi r^k} \sum_{j-1}^{2k} (-1)^j\,\mathrm{Re}(G(r\bar{e}^{\,ij\pi/k})), \tag{4}$$

just as in Theorem 1, so that it only remains to determine the error bound.

The framework above can also be regarded as a special case of a sequence $\{a_k: -\infty < k < \infty\}$ with $\sum_{k=-\infty}^{\infty} |a_k| < \infty$. (In particular, let $a_k = q_k r^k$ with $0 < r < 1$ for $k \geqslant 0$ and $a_k = 0$ for $k < 0$.)

We then can consider the Fourier transform

$$\phi(u) = \sum_{k=-\infty}^{\infty} a_k\,e^{iku}, \tag{5}$$

which has an inverse

$$a_k = \frac{1}{2\pi} \int_0^{2\pi} \phi(u)\,e^{-iku}\,du, \tag{6}$$

as can easily be verified by substituting (5) into (6); see p.511 of Feller [5]. With $a_k = q_k r^k$ for $k \geqslant 0$ and $a_k = 0$ for $k < 0$, (6) reduces to (3).

The error bound for the trapezoidal rule approximation to (6) now follows from the discrete Poisson summation formula.

Theorem 2 (discrete Poisson summation formula). *For integers k and $m > 0$,*

$$a_k = \frac{1}{m} \sum_{j=0}^{m-1} \phi(2\pi j/m)\,e^{-i2\pi jk/m} - \sum_{\substack{j=-\infty \\ j \neq 0}}^{\infty} a_{k+jm}.$$

Proof of Theorem 2. Given k and m, form the periodic sequence with terms

$$a_k^p = \sum_{j=-\infty}^{\infty} a_{k+jm}. \tag{7}$$

(The series in (7) converges absolutely since $\sum_{j=-\infty}^{\infty} |a_j| < \infty$.) Next construct the discrete Fourier transform of $\{a_k^p\}$, see p.51 of Rabiner and Gold [12], to obtain

$$\hat{a}_k^p = \frac{1}{m} \sum_{j=0}^{m-1} a_j^p\,e^{i2\pi kj/m}$$
$$= \frac{1}{m} \sum_{j=0}^{m-1} \sum_{l=-\infty}^{\infty} a_{j+lm}\,e^{i2\pi jk/m}$$
$$= \frac{1}{m} \sum_{j=-\infty}^{\infty} a_j\,e^{i2\pi jk/m} = \frac{1}{m} \phi\left(\frac{2\pi k}{m}\right).$$

Finally, from the inversion formula for discrete Fourier transforms,

$$a_k^p = \sum_{j=0}^{m-1} \hat{a}_j^p \, e^{-i2\pi jk/m}$$
$$= \frac{1}{m} \sum_{j=0}^{m-1} \phi(2\pi j/m) \, e^{-i2\pi jk/m}. \quad \square$$

Theorem 2 implies that the trapezoidal rule approximation to (6) with step size $2\pi/m$ has discretization error

$$e_d = \sum_{\substack{j=-\infty \\ j \neq 0}}^{\infty} a_{k+jm}. \tag{8}$$

For the special case of $a_k = q_k r^k$ for $k \geqslant 0$ and $a_k = 0$ for $k < 0$,

$$e_d = \sum_{j=1}^{\infty} a_{k+jm} = \sum_{j=1}^{\infty} (q_{k+jm}) r^{k+jm} \tag{9}$$

so that

$$|e_d| \leqslant \frac{r^{k+m}}{1 - r^m}. \tag{10}$$

When we focus on q_k, we divide (10) by r^k and obtain the error bound $r^m/(1 - r^m)$, which yields Theorem 1 when we set $m = 2k$ as in (4). We obtain the last equality in Theorem 1 because $\mathrm{Re}(G(z)) = \mathrm{Re}(G(\bar{z}))$.

3. The M/M/1 example

The number of customers served in a busy period of an M/M/1 queue with traffic intensity ρ has a probability mass function

$$p_k = \frac{1}{k} \binom{2k-2}{k-1} \rho^{k-1} (1+\rho)^{-2k+1}, \quad k \geqslant 1, \tag{11}$$

and probability generating function

$$P(z) \equiv \sum_{k=0}^{\infty} p_k z^k = \frac{1 - \sqrt{1 - \beta z}}{\sqrt{\beta\rho}}, \tag{12}$$

where $\beta = 4\rho/(1+\rho)^2$; see p.65 of Riordan [13]. The tail probabilities

$$q_k = p_{k+1} + p_{k+2} + \cdots \tag{13}$$

thus have generating function

$$G(z) \equiv \sum_{k=0}^{\infty} q_k z^k = \frac{1 - P(z)}{1 - z} \tag{14}$$

for $P(z)$ in (12).

The displayed program in Section 1 computes q_k to an accuracy of 10^{-8} in the case $\rho = 0.75$. The real part of $G(z)$ for any z is computed in lines 80–84. The damping parameter r is set equal to $10^{-\gamma/2k}$ to achieve accuracy $10^{-\gamma} \equiv 10^{-E} = 10^{-8}$ in lines 21–22. The sum in Theorem 1 is computed in lines 30–34.

Table 1
A comparison of numerical-inversion and asymptotic approximations with exact values of p_k and q_k in (11) and (13)

k	p_k			q_k		
	exact values from (11)	(inversion − exact) $\times 10^{10}$ for $E = 7$	(asymp − exact) ÷ exact from (15)	exact values from (13)	(inversion − exact) $\times 10^{10}$ for $E = 7$	(asymp − exact) ÷ exact from (16)
1	0.571428571	69	−0.44	0.428571429	220	
2	0.139941691	21	−0.20	0.288629738	128	
3	0.068542869	11	−0.13	0.220086869	87	
4	0.041965022	7	−0.10	0.178121847	66	
5	0.028776015	4	−0.08	0.149345832	51	
10	0.008803257	1	−0.04	0.079604889	20	
20	0.002483026		−0.02	0.035708032	5	
40	0.000575657		−0.009	0.012072949	1	1.27
80	0.000088790		−0.005	0.002492008		0.70
160	0.000006017		−0.002	0.000208294		0.38
240	0.000000629		−0.002	0.000023794		0.27
320	0.000000078		−0.001	0.000003121		0.21
400	0.000000011		−0.001	0.000000443		0.17

As indicated in Remark 5 above, the transform can be used to determine the asymptotic behavior of p_k and q_k as $k \to \infty$. In particular, from (12) and p. 150 of Wilf [14] or p. 498 of Bender [2], we find that

$$p_k \sim \alpha_k \equiv -\frac{1}{\sqrt{\beta\rho}} \frac{\beta^k}{k^{3/2}\Gamma(-1/2)} = \frac{\beta^k}{2\sqrt{\beta\rho\pi k^3}}, \tag{15}$$

where $p_k \sim \alpha_k$ means that $p_k/\alpha_k \to 1$ as $k \to \infty$, which agrees with what we get from (11) by applying Stirling's formula. Moreover, from (14) we obtain

$$q_k \sim \frac{\alpha_k}{\beta^{-1} - 1} = \frac{4\rho}{(1-\rho)^2}\alpha_k \tag{16}$$

for α_k in (15).

Table 1 compares the exact values of p_k and q_k based on (11) and (13) with the numerical inversion based on Theorem 1 and the asymptotic values from (15) and (16). From Table 1, we see that the asymptotics do not become accurate too quickly, but they become accurate before the calculation becomes difficult. It is interesting that the asymptotics are much better for the probability mass function values p_k than for the complementary cumulative distribution function values q_k. (Similar behavior holds for the continuous-time length of the M/M/1 busy period.) Finally, note that the numerical inversion consistently achieves the prescribed 10^{-7} accuracy.

4. Conclusion

We have applied the discrete Poisson summation formula (Theorem 2) to characterize the discretization error associated with the trapezoidal-rule method for numerically integrating standard inversion integrals for generating functions ((3) and (6)). For most operations research applications, sufficient accuracy (e.g., 10^{-8}) is obtained with a very manageable computation (Theorem 1). Similar methods also can be used to numerically invert other transforms but easily computable error bounds are usually not available; see [1]. In summary, we believe that numerical transform inversion deserves a more prominent place in the operations research toolkit. (However, we do not make strong claims of originality, because these techniques are classical, and variants of our algorithm LATTICE − POISSON were previously proposed by others.)

Acknowledgment

We thank Dimitris Bertsimas, Bharat Doshi, Kerry Fendick, Daniel Heyman, Toshio Hosono, David Jagerman and Henk Tijms for assistance. We thank Kerry Fendick for writing the C++ program implementing LATTICE-POISSON.

References

[1] J. Abate and W. Whitt, "The Fourier-series method for inverting transforms of probability distributions", *Queueing Systems* **10**, 5–88 (1992).
[2] E.A. Bender, "Asymptotic methods in enumeration", *SIAM Rev.* **16**, 485–515 (1974).
[3] J.K. Cavers, "On the fast Fourier transform inversion of probability generating functions", *J. Inst. Math. Appl.* **22**, 275–282 (1978).
[4] J.N. Daigle, "Queue length distributions from probability generating functions via discrete Fourier transforms", *Oper. Res. Lett.* **8**, 229–236 (1989).
[5] W. Feller, *An Introduction to Probability Theory and its Applications*, Vol. II, second ed., Wiley, New York, 1971.
[6] T. Hosono, "Numerical algorithms for Taylor series expansion", *Electron. Commun. Japan* **69**, 10–18 (1986).
[7] D.L. Jagerman, "An inversion technique for the Laplace transform", *Bell System Tech. J.* **61**, 1995–2002 (1982).
[8] D.L. Jagerman, MATHCALC, AT & T Bell Laboratories, Holmdel, NJ, 1987.
[9] Y. Kida, "UBASIC: Version 8.12", Faculty of Science, Kanazawa University, 1-1 Marunouchi, Kanazawa 920, Japan, 1990.
[10] J.N. Lyness, "Differentiation formulas for analytic functions", *Math. Computation* **22**, 352–362 (1968).
[11] W.D. Neumann, "UBASIC a public-domain BASIC for mathematics", *Notices Amer. Math. Soc.* **36**, 557–559 (1989).
[12] L.R. Rabiner and B. Gold, *Theory and Application of Digital Signal Processing*, Prentice-Hall, Englewood Cliffs, NJ, 1975.
[13] J. Riordan, *Stochastic Service Systems*, Wiley, New York, 1962.
[14] H.S. Wilf, *Generatingfunctionology*, Academic, New York, 1990.