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Some Remarks on the Numerical Evaluation of Fourier and Fourier-Bessel Transforms

FREDERIC MANDEL

Department of Chemistry, University of Kansas, Lawrence, Kansas 66044

and

Department of Chemistry, Rice University, Houston, Texas 77001

AND

RICHARD J. BEARMAN

Department of Chemistry, University of Kansas, Lawrence, Kansas 66044

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Numerous special techniques have been proposed for the numerical evaluation of Fourier transform integrals. Two of these techniques, a method proposed by Broyles based on the trapezoidal rule and one due to Filon, are compared. Also the efficacy of an algorithm proposed by Cooley and Tukey for doing Fourier sums rapidly is discussed and it is shown how this algorithm may be applied to the above Fourier transform techniques. Finally, the numerical evaluation of Fourier–Bessel transforms is discussed.

I. INTRODUCTION

The numerical integration of the three-dimensional Fourier transform integrals, e.g.,

$$\hat{f}(k) = 4\pi \int_0^\infty f(r)(r/k) \sin kr \, dr, \tag{1a}$$

and

$$f(r) = \frac{1}{2\pi^2} \int_0^\infty \hat{f}(k)(k/r) \sin kr \, dk, \tag{1b}$$

is beset with difficulties. For large k, the graph of $rf(r) \sin kr$ consists of positive and negative areas of nearly equal size. The addition of these two areas results

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in substantial cancellation with a consequent loss of accuracy. Furthermore, for large k, the function oscillates very rapidly, necessitating the use of very fine grid spacing.

Because of the widespread occurrence and usefulness of Fourier transforms, many special techniques have been proposed for their numerical evaluation [1]. It is the objective of this paper to compare two of the techniques and to discuss the errors associated with them.

II. The Broyles Modification of The Trapezoidal Rule

The first technique is based on the trapezoidal rule and has recently been proposed by Broyles [2]. Broyles has shown that when the upper limits of integration are truncated to $(N-1)\hat{r}$, and the integrals in Eqs. (1a) and (1b) are replaced by the sums

$$\hat{f}(k) = \hat{f}(m\hat{k}) = \frac{4\pi\hat{r}^2}{m\hat{k}} \sum_{n=0}^{N-1} n f(n\hat{r}) \sin(nm\hat{r}\hat{k}), \tag{2a}$$

and

$$f(r) = f(n\hat{r}) = \frac{\hat{k}^2}{2\pi^2 n\hat{r}} \sum_{m=0}^{N-1} m\hat{f}(m\hat{k}) \sin(nm\hat{r}\hat{k}), \tag{2b}$$

then the inverse of $\hat{f}(r)$ from Eq. (2b) agrees exactly, within calculational errors, with the original given $f(r)$, provided that

$$\hat{r}\hat{k} = \frac{2\pi}{2N-1}, \tag{3}$$

where $\hat{r}$ and $\hat{k}$ are the grid size for r and k, respectively, and N is the number of grid points.

To check the accuracy of this method, we have numerically evaluated the Fourier sine transform of the function

$$c(x) = \begin{cases} x^2 & 0 \leqslant x \leqslant 2\pi \\ 0 & x > 2\pi, \end{cases} \tag{4a}$$

which may also be analytically evaluated with the aid of the integral

$$\int_0^{2\pi} x^3 \sin kx \, dx = \frac{12\pi^2k^2 - 6}{k^4} \sin 2\pi k - \frac{[8\pi^3k^2 - 12\pi]}{k^3} \cos 2\pi k. \tag{4b}$$

In Table I, we give the exact transform of $c(x)$ and compare it with the value obtained from Eqs. (2a) and (3) on a GE 635 computer using a Fortran IV, single-precision program with $\hat{r} = 0.01\pi$, $N = 201$. Using Eq. (2b), we have then inverted the resulting transforms in an attempt to regain the original function. These results are tabulated in the first three columns of Table II. Although the inverse Fourier

TABLE I

The Fourier Sine Transform of $c(x)$ Multiplied by $k/4\pi$

k	Exact value	Numerical transform[a]
0.49875	196.444	196.465
2.4938	97.7026	97.8047
4.9875	−49.6505	−49.8547
9.9751	−24.7105	−25.1187
20.4489	11.5951	12.4298
34.9127	−6.1128	−7.5292
49.875	−3.5569	−5.5623
75.810	−1.2328	−4.2271
99.751	0.02207	−3.9256

[a] Eq. (2a) and (3) were used to evaluate the transform.

transform agrees quite well with the original function, significant discrepancies appear at large k for the transform itself. Hence, forcing the inverse transform to agree with the starting function does not necessarily lead to acceptable values for the transform. In the next section, we consider another technique which does not have enforced consistency, but which does appear to have superior accuracy under some circumstances.

III. Filon's Method

The second technique was proposed by Filon [1, 3]. Filon's method requires the approximation of $g(r) \equiv rf(r)$ by a parabola and then an integration by parts. This procedure yields for a finite interval of integration

$$\int_a^b g(r) \sin kr \, dr \simeq h\{-\alpha[g(b) \cos kb - g(a) \cos ka] + \beta S_{2n} + \gamma S_{2n-1}\}, \quad (5)$$

TABLE II

A Comparison of the Inverse Fourier Sine Transform of $\hat{c}(k)$ with $c(x)$

x	x^2	Eq. (2b)	Eq. (14)
0.15707	0.0246740	0.0251305	0.0241296
0.50265	0.2526619	0.2527272	0.2525220
1.0996	1.209026	1.209058	1.209089
1.5707	2.467401	2.467450	2.467306
2.0106	4.042590	4.042555	4.042593
2.9531	8.720784	8.720830	8.720793
3.8013	14.45009	14.45009	14.45005
4.8381	23.40676	23.40678	23.40676
5.3721	28.85972	28.85972	28.85970
6.2203	38.69282	38.69290	38.69279

where

$$S_{2n} = \tfrac{1}{2} g(a) \sin ka + g(a + 2h) \sin k(a + 2h) + \cdots + \tfrac{1}{2} g(b) \sin kb, \tag{6}$$

$$S_{2n-1} = g(a + h) \sin k(a + h) + g(a + 3h) \sin k(a + 3h) + \cdots + g(b - h) \sin k(b - h), \tag{7}$$

$$\theta = kh = \frac{k(b - a)}{2N},$$

$$\alpha = \alpha(\theta) = \frac{\theta^2 + \theta \sin \theta \cos \theta - 2 \sin^2 \theta}{\theta^3},$$

$$\beta = \beta(\theta) = \frac{2[\theta(1 + \cos^2 \theta) - 2 \sin \theta \cos \theta]}{\theta^3}, \tag{8}$$

and

$$\gamma = \gamma(\theta) = \frac{4(\sin \theta - \theta \cos \theta)}{\theta^3}. \tag{9}$$

In Table III, we compare the exact Fourier sine transform of $c(x)$ of Eq. (4) with the Filon value and with the Broyles value for a number of points, for variety, mostly different from those of Table I, but within the same range. In Table IV, a comparison is made for the function

$$d(x) = \begin{cases} \cos x & 0 \leqslant x \leqslant 2\pi \\ 0 & x > 2\pi. \end{cases} \tag{9a}$$

The exact value is obtained from

$$\int_0^{2\pi} x \cos x \sin kx \, dx = \frac{-2\pi k}{k^2 - 1} \cos 2\pi k + \frac{1}{2} \left\{ \frac{\sin 2\pi(k-1)}{(k-1)^2} + \frac{\sin 2\pi(k+1)}{(k+1)^2} \right\}. \tag{9b}$$

From these tables, it appears that the two methods are of similar accuracy for sine transforms with $k < 10$. Broyle's technique is somewhat faster computationally. For large k's, Filon's method is appreciably better.

TABLE III

The Fourier Sine Transform of $c(x)$ Multiplied by $k/4\pi$

k	Exact value	Filon[a]	Broyles[b]
0.49875	196.444	196.448	196.465
1.9950	−120.449	−120.449	−120.531
3.9900	−61.918	−61.918	−62.081
5.9850	−41.397	−41.397	−41.642
10.474	23.507	23.507	23.936
20.948	−11.289	−11.289	−12.144
40.399	4.9872	4.9872	6.6211
75.810	−1.2328	−1.2328	−4.2271
99.751	−0.2207	−0.02210	−3.9256

[a] $h = \hat{r}$.
[b] $\hat{r}$, $\hat{k}$, N as in Table 1.

TABLE IV

The Fourier Sine Transform of $d(x)$
Multiplied by $k/4\pi$

k	Exact value	Filon	Broyles
0.49875	−4.13662	−4.15405	−4.15343
1.9950	−4.23936	−4.22178	−4.22385
3.9900	−1.68649	−1.68173	−1.68586
5.9850	−1.08090	−1.07805	−1.08424
7.9800	−0.79776	−0.79571	−0.80396
10.474	0.60031	0.59877	0.60960
15.461	0.39815	0.39713	0.41310
20.948	−0.28599	−0.28526	−0.30685
30.424	0.18457	0.18408	0.21533
40.399	0.12605	0.12569	0.16697
50.873	−0.08671	−0.08643	−0.13808
75.810	−0.03107	−0.03091	−0.10655
99.751	-4.586×10^{-3}	-3.586×10^{-3}	-9.894×10^{-1}

IV. Fast-Fourier-Transform

Recently, Cooley and Tukey [4] have devised an algorithm, which we shall call "fast-Fourier-transform," whereby sums of the form

$$\hat{a}(m) = \sum_{n=0}^{M-1} a(n) \exp[2\pi inm/M], \tag{10}$$

can be computed considerably more rapidly than by previous techniques provided $M = 2^l$ and l is an integer. Library subroutine programs to evaluate Eq. (10) have been written and are available from both IBM (Fort) and General Electric (RLFORT). Hence, one would like to use these programs to perform the summations in Filon's method or Broyles' method.

Rasaiah and Friedman [5] have shown that it is possible to use the fast-Fourier-transform technique to calculate the sums in Eqs. (2a) and (2b) although there are several difficulties involved. First, $M = 2^l$ has to be even while $2N - 1$ is odd. Thus, the argument of the sine function in Eq. (10) contains $M = 2N$ instead of $2N - 1$ which causes an error of $1/M$ in the resulting transforms (see Ref. [5]). Secondly, Eq. (10) consists of $M - 1$ terms while Eq. (2) has only $N - 1$ terms.

As an alternative to the method of Rasaiah and Friedman, we may propose the following approach. We substitute Eq. (2b) into Eq. (2a) and find

$$\begin{aligned} f(m\hat{k}) &= \frac{4\pi\hat{r}^2}{m\hat{k}} \sum_{n=0}^{N-1} \frac{n\hat{k}^2}{2\pi^2 n\hat{r}} \sum_{m'=0}^{N-1} m' \hat{f}(m'\hat{k}) \sin(nm'\hat{r}\hat{k}) \sin(nm\hat{r}\hat{k}) \\ &= \frac{2\hat{r}\hat{k}}{m\pi} \sum_{m'=0}^{N-1} m' \hat{f}(m'\hat{k}) \sum_{n=0}^{N-1} \sin(nm'\hat{r}\hat{k}) \sin(nm\hat{r}\hat{k}). \end{aligned} \tag{11}$$

Broyles has shown that setting the second sum in Eq. (11) proportional to the kronecker delta $\delta mm'$ leads to Eq. (3), and to the inverse of a transform equal to the original function. However, the Euler–Maclaurin sum formula [6]

$$\int_a^b f(x)\, dx = T_r + \sum_{m=1}^{n-1} \frac{(-)^m B_m (\Delta x)^{2m}}{(2m)!} f^{(2m-1)}(x) \Big|_a^b + R_n, \tag{12}$$

where

$$R_n = \frac{(\Delta x)^{2n+1}}{(2n)!} \int_0^1 \phi_{2n}(t) \sum_{m=0}^{r-1} f^{(2n)}(a + m\Delta x + t\Delta x)\, dt,$$

T_r is the r-point trapezoidal rule sum, the B_n are the Bernoulli numbers and $f^{(n)}(x)$ is the n-th derivative of $f(x)$, may be used to replace the sum by an integral.

Recalling that for a periodic function $f^{(n)}(a) = f^{(n)}(b)$, and neglecting the remainder term R_n, Eq. (12) may be rewritten

$$\hat{f}(m\hat{k}) = \frac{2\hat{r}\hat{k}}{m\pi} \sum_{m'=0}^{N-1} m'\hat{f}(m'\hat{k}) \int_0^{N-1} \sin(nm\hat{r}\hat{k}) \sin(nm'\hat{r}\hat{k})\, dn. \tag{13}$$

The orthogonality of the integral leads to the following expression for the product $\hat{r}\hat{k}$:

$$\hat{r}\hat{k} = \frac{\pi}{N-1} = \frac{2\pi}{2N-2}. \tag{14}$$

To see whether Eq. (14) is appreciably inferior to Eq. (3) of Broyles, we have tabulated the inverse Fourier transform of the function of Eq. (4a), using Eq. (14), in the last column of Table 2. Comparison of columns 3 and 4 demonstrates that Eq. (14) can lead to results comparable in consistency with those from Eq. (3).

The advantage of the approximation of Eq. (14) is that, for real $f(r)$, Eq. (2a) can be evaluated by the fast-Fourier-transform technique, as can be seen by substituting into the imaginary part of Eq. (10):

$$M = 2N - 2 = 2^l, \tag{15}$$

$$\begin{aligned} a(n) &= nf(\hat{n}\hat{r}), & 0 \leqslant n \leqslant N-1 \\ a(n) &= 0, & N \leqslant n \leqslant 2N-2. \end{aligned} \tag{16}$$

Next we shall show how the fast-Fourier-transform may be used to do the sums in Filon's method, albeit at the cost of arbitrary grid spacing.

Setting $M = 2N = 2^l$ and $\hat{r}\hat{k} = 2\pi/M$, where $\hat{r} = h$ and $k = m\hat{k}$ and letting the lower limit of Eq. (5) equal zero, we can rewrite Eq. (5) as

$$\begin{aligned} \int_0^b g(r) \sin kr\, dr \cong{}& h\{\alpha[g(0) - g(b)\cos kb]\} \\ &+ \gamma \sum_{n=0}^{M-1} g(n\hat{r}) \sin(2\pi nm/M) \\ &+ (\beta - \gamma) \sum_{n=0}^{N-1} g(2n\hat{r}) \sin(2\pi nm/N) + \frac{\beta}{2} g(b) \sin kb. \end{aligned} \tag{20}$$

The sums in Eq. (17) are of the form of Eq. (10), and hence the fast-Fourier-transform may be employed. The use of the fast-Fourier-transform in the Filon method results in a computational time which is greater than the time for the trapezoidal rule. We conclude that the trapezoidal rule is preferable for sine transforms with small values of k, while Filon's rule should be used for large values of k, provided that in practice the Filon result remains more accurate using the fast-Fourier-technique.

IV. Fourier-Bessel Transforms

In this section we discuss the numerical evaluation of Fourier–Bessel transforms. We shall define the Fourier–Bessel transform

$$\hat{f}_n(k) = \int_0^\infty r^2 f_n(r) j_n(kr)\, dr, \tag{18}$$

TABLE V

The nth Order Fourier-Bessel Transform[a]

r	Original function	$n = 0$	$n = 2$	$n = 4$	$n = 6$
0.05	−15.347577	−15.347571	−11.359	−1.937	−0.185
0.50	−8.4084868	−8.4084870	−8.488	−8.269	−8.521
0.95	−3.1859760	−3.1859759	−3.175	−3.225	−3.149
1.00	−2.7787678	−2.7787678	−2.789	−2.743	−2.812
1.05	0.0	3.4×10^{-8}	9.2×10^{-3}	-3.2×10^{-2}	-3.1×10^{-2}
2.00	0.0	1.6×10^{-8}	-2.7×10^{-3}	9.4×10^{-3}	-9.1×10^{-2}
3.00	0.0	1.4×10^{-8}	-1.3×10^{-3}	4.6×10^{-3}	-4.4×10^{-3}
4.00	0.0	8.7×10^{-10}	-8.2×10^{-4}	2.9×10^{-3}	-2.8×10^{-3}
5.00	0.0	3.8×10^{-9}	-6.2×10^{-4}	2.2×10^{-3}	-2.1×10^{-2}

[a] The nth order Fourier-Bessel transform of the original function was performed. The resulting function was then transformed again in an attempt to regain the original function.

where $j_n(kr)$ is the spherical Bessel function of order n and is related to the ordinary Bessel function $J_n(kr)$ as follows

$$j_n(x) = \left(\frac{\pi}{2x}\right)^{1/2} J_{n+1/2}(x). \tag{19}$$

The inverse transform is

$$f_n(r) = \frac{2}{\pi} \int_0^\infty k^2 \hat{f}_n(k) j_n(kr) dk. \tag{20}$$

Except for the $n = 0$ case, when $j_n(x) = \sin x/x$, the spherical Bessel functions contain cosine terms, and utilization of the Broyles' trapezoidal rule may not result in accurate transforms. To test the accuracy of his rule, we used it to evaluate the first four even spherical Bessel transforms of the function tabulated in the first column of Table V [7]. We then inverted these transforms to regain the original function [8]. The results are tabulated in Table V. It is obvious from Table V that the transforms obtained by using the Broyles' rule grow progressively worse as the order of the spherical Bessel function increases. We note that Filon's rule cannot be applied to the spherical Bessel functions. It would seem, therefore, that special numerical techniques are required for Fourier-Bessel transforms [9].

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