Letter to the Editors

On the Accuracy of Numerical Fourier Transforms

Since the availability of the "fast" Fourier transform routine [1], there have been many works on the numerical Fourier transform schemes [2–5]. A recent paper by Abramovici [5], among other things, seemed to show that Filon's method is poor in evaluating the transform

$$\phi(\omega) = \int_0^T f(t) \, e^{i\omega t} \, dt, \qquad (1)$$

for large values of ω , even when f(t) is reasonably smooth. From the derivation of Filon's formula, we expect that, except for some special cases, it should be superior to the trapezoidal or Simpson's rule for *large* values of ω . The reason is that the errors in Filon's method [6] are proportional to the derivatives of f(t)itself instead of $f(t) \sin \omega t$ or $f(t) \cos \omega t$ and are therefore relatively independent of ω . It is the purpose of this note to show that one of the test functions used in [5] was a special case for which the trapezoidal rule is anomalously accurate, and that a computational error gave rise to erroneously bad Filon results for the other function.

Filon's formula for the Fourier sine transform is

$$\phi_{t}(\omega) = \int_{0}^{T} f(t) \sin \omega t \, dt$$

$$\simeq \Delta t \{ \alpha [f(0) - f(T) \cos(\omega T)] + \beta S_{2n} + \gamma S_{2n-1} \}, \qquad (2)$$

where α , β , γ , S_{2n} , S_{2n-1} , etc., are defined in many places [3, 6]. We have applied the formula to the function

$$f(t) = t \cos \omega_0 t, \tag{3}$$

with $T = 2\pi$, $\omega_0 = 1$ and 50. Results are given in Tables I and II. The numbers are in substantial disagreement with the corresponding numbers in Tables I and II of Abramovici's paper [5]. Incidentally, if the sign of the term $f(T)\cos(\omega T)$ in Eq. (2) is reversed, Abramovici's numbers will be obtained. The results in Tables I and II confirm the expected accuracy of Filon's method.

TABLE I

Values of $\phi_I(\omega) = \int$	$\int_{0}^{T} f(t) \sin \omega t dt$
for $f(t) = t \cos \omega_0 t$	$\omega_0=1, T=2\pi.$

ω	Exact value	No. of integration points	Filon
1	-1.57079632679		
-		64	-1.570 81335274
		256	-1.5707963 9330
		1024	-1.57079632 705
		2048	-1.5707963268 2
30	$-2.09672479661 \times 10^{-1}$		
		64	-2.09 737961629 × 10 ⁻¹
		256	-2.0967247 8623 $ imes$ 10 ⁻¹
		1024	-2.096724796 56 $ imes$ 10 ⁻¹
		2048	$-2.09672479661^a \times 10^{-1}$
100	$-6.2838136885 \times 10^{-2}$		
		256	$-6.28381 \mid 40629 \times 10^{-2}$
		1024	-6.283813688 4 $ imes$ 10 ⁻²
		2048	$-6.2838136885^{a} imes 10^{-2}$
500	$-1.25664208800 imes 10^{-2}$		
		1024	-1.256642 12111 $ imes$ 10 ⁻²
		2048	$-1.25664208800^a \times 10^{-2}$

^a Accurate to all digits shown.

Our Filon results for the cosine transform of (3) with $\omega_0 = 50$ essentially agree to the values in Table III of Abramovici's paper. It happens that the cosine transform

$$\phi_R(\omega) = \int_0^T f(t) \cos \omega t \, dt, \quad f(t) = t \cos \omega_0 t, \quad T = 2\pi \tag{4}$$

is a special case where the trapezoidal rule is practically exact no matter whether

TABLE II

Values of $\phi_I(\omega) = \int_0^T f(t) \sin \omega t dt$
for $f(t) = t \cos \omega_0 t$, $\omega_0 = 50$, $T = 2\pi$.

		No. of integration	
ω	Exact value	points	Filon
1	2.51427983481 × 10 ⁻³		
		256	2. 383038517 $ imes$ 10 ⁻³
		1024	2.51 3901562 $ imes$ 10 ⁻³
		2048	$2.5142 \mid 56523 imes 10^{-3}$
30	1.17809724510 × 10 ⁻¹		αδ
		256	$1.1 \mid 21968687 \times 10^{-1}$
		1024	$1.177 \mid 921769 imes 10^{-1}$
		2048	1.1780 86350 × 10 ⁻¹
100	$-8.37758040957 \times 10^{-2}$		
		256	$-7.036141929 \times 10^{-2}$
		1024	-8.37 6469805 \times 10 ⁻²
		2048	$-8.3775 \mid 04964 \times 10^{-2}$
500	$-1.26933036509 \times 10^{-2}$		
		1024	-1.2 56651002 \times 10 ⁻²
		2048	$-1.26933 \mid 2502 \times 10^{-2}$

the "linear trend" is subtracted out or not. The well-known trapezoidal rule is

$$\phi(\omega) = \int_0^T f(t) e^{i\omega t} dt$$

$$\simeq \Delta t \left\{ \frac{1}{2} \left[-f(0) + f(T) e^{i\omega T} \right] + \sum_{j=0}^{N-1} f(t_j) e^{i\omega t_j} \right\}$$
(5)

where

$$t_j = j \Delta t = jT/N, \quad j = 0, 1, ..., N.$$

It is true that the "fast" Fourier transform routine can only evaluate the sum

$$\Delta t \sum_{j=0}^{N-1} f(t_j) e^{i\omega t_j} \tag{6}$$

for some discrete values of ω , it is a simple matter to add the correction to (6) to yield the sum in (5). Of course, Abramovici's "trapezoidal *FFT*" method makes the correction term unnecessary.

Values of FFT as shown in Table III of [5] for comparison are poor. The improvement of the FFT results by the trapezoidal FFT method is tremendous. However, when Eq. (5) is used instead of (6), exactly the same accuracy is obtained. The accuracy here is due to a special feature of the integrand of (4).

According to the Euler-Maclaurin formula [7, 8], if the integrand is analytic and the odd-order derivatives are equal at the end points, the truncation error of the trapezoidal rule is practically zero. This condition is satisfied by the integrand of (4) when both ω and ω_0 are integers. The following proof is due to Dr. R. Coldwell.

The integrand of (4) is

$$t\cos\omega_0 t\cos\omega t = \frac{t}{2}\left[\cos(\omega_0 + \omega) t + \cos(\omega_0 - \omega) t\right]. \tag{7}$$

The first term is of the form

$$g(t) = t \cos nt, \quad n = \omega_0 + \omega = \text{integer},$$
 (8)

so

$$g(2\pi + t) = 2\pi \cos nt + t \cos nt.$$

Consequently, all odd derivatives of g(t) at t = 0 and $t = 2\pi$ are equal. The same conclusion holds also for the second term of (7) when $\omega_0 \neq \omega$. When $\omega_0 = \omega$, the second term is simply t/2, and the trapezoidal rule is, of course, exact.

The arguments following Eq. (8) can be used to show that the trapezoidal rule is practically exact for the finite cosine transform of a linear function $f(t) = c_1 t + c_2$ for all discrete values of ω defined in Eq. (4) of [5], the reason being that the integrand $g(t) = f(t) \cos \omega t$ satisfies $g(T + t) - g(t) = Tc_1 \cos \omega t$ and therefore $g^{(n)}(0) = g^{(n)}(T)$ for all odd numbers *n*. The linear trend defined in Eq. (7) of [5] is of course a linear function of *t*. This explains the fact that the trapezoidal *FFT* method and the usual trapezoidal rule are equally accurate for the cosine transform (4). Some other examples with the above mentioned property include

(i)
$$\int_0^\infty e^{-\alpha t^2} \cos \omega t \, dt$$
,
(ii) $\int_0^\infty t e^{-\alpha t^2} \sin \omega t \, dt$,
(iii) $\int_0^\infty \frac{t \sin \omega t}{(t^2 + \alpha^2)^2} \, dt$.

Although Filon's method is as accurate as usual for these cases, the trapezoidal rule or the trapezoidal *FFT* method is anomously accurate.

References

- 1. J. W. COOLEY AND J. W. TUKEY, Math. Comp. 19 (1965), 297.
- 2. J. C. RASAIAH AND H. L. FRIEDMAN, J. Chem. Phys. 48 (1968), 2742.
- 3. F. MANDEL AND R. J. BEARMAN, J. Comp. Phys. 7 (1971), 637.
- 4. F. LADO, J. Comp. Phys. 8 (1971), 417.
- 5. F. ABRAMOVICI, J. Comp. Phys. 11 (1973), 28.
- 6. M. ABRAMOWITZ AND I. A. STEGUN, "Handbook of Mathematical Functions," p. 890, Dover, New York, 1965.
- 7. M. ABRAMOWITZ AND I. A. STEGUN, "Handbook of Mathematical Functions," p. 886, Dover, New York, 1965.
- 8. A. RALSTON, "A First Course in Numerical Analysis," p. 133, McGraw-Hill, New York, 1965.

RECEIVED: December 18, 1973

KIN-CHUE NG

Department of Physics University of Florida Gainesville, Florida 32611