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NOTE

Methods for the Numerical Evaluation of Fourier Integrals[1]

In many problems, Fourier transforms of the form

$$\Phi(\omega) = \int_0^\infty f(t)\cos(\omega t)\,dt \tag{1}$$

must be evaluated numerically. Some methods have been used to treat this problem with limited success [1]–[4]. The method introduced here has also been successfully employed in certain applications [5]. In this method, the domain of integration is partitioned into two regions: $0 \leqslant t \leqslant t_m$ and $t_m \leqslant t \leqslant \infty$, designated as the near region and asymptotic region, respectively. The Fourier integral can then be written as $\Phi(\omega) = I(\omega, t_m) + J(\omega, t_m)$, where I and J are the near and asymptotic contributions, respectively. The different methods of evaluating the terms I and J, are discussed below.

A. *Near Region*

Let $\{t_i\}$, $i = 1, 2 \cdots m$, be a proper net (subdivision) on the interval $\{0, t_m\}$. Then

$$I = \sum_{i=1}^{m-1} I_i\,, \qquad \text{where} \quad I_i = \int_{t_i}^{t_{i+1}} f(t)\cos(\omega t)\,dt. \tag{2}$$

Different techniques can be used to approximate the elements $\{I_i\}$. Commonly, $f(t)$ is approximated in the interval (t_i, t_{i+1}) by a simple function whose product with $\cos(\omega t)$ is readily integrable in closed form. Hastrup [4] has used a linear function, and Filon [1] has used a quadratic. Since $f(t)$ must be monotone-decreasing over much of its domain, the behavior of such functions can often be better approximated by simple exponentials over limited regions. Thus, one may write $f(t) \simeq g(t) = \alpha_i \exp(\beta_i t)$ for $(t_i \leqslant t \leqslant t_{i+1})$ where the values of the parameters α_i and β_i are fixed by the conditions $g(t) = f(t)$ at $t = t_i$ and t_{i+1}. The exponential approximation yields

$$I_i = \frac{\alpha_i}{\beta_i^2 + \omega^2}\{e^{\beta_i t_{i+1}}[\beta_i \cos(\omega t_{i+1}) + \omega \sin(\omega t_{i+1})] - e^{\beta_i t_i}[\beta_i \cos(\omega t_i) + \omega \sin(\omega t_i)]\}. \tag{3}$$

[1] Work performed under the auspices of the U.S. Atomic Energy Commission.

For slowly varying $f(t)$, an alternative approach employs the law of the mean. Applying the mean-value theorem to Eq. (2), one can write

$$I_i = f(\bar{t}) \int_{t_i}^{t_{i+1}} \cos(\omega t)\, dt = \frac{f(\bar{t})}{\omega} [\sin(\omega t_{i+1}) - \sin(\omega t_i)], \tag{4}$$

where $\bar{t}$ is some value of t in the interval (t_i, t_{i+1}). Application of the mean-value theorem implies that the zeros of $\cos(\omega t)$ must be a subset of $\{t_i\}$. The two simplest approximations for slowly varying $f(t)$ are $f(\bar{t}) \cong f[\frac{1}{2}(t_i + t_{i+1})]$ or $f(\bar{t}) \cong \frac{1}{2}[f(t_i) + f(t_{i+1})]$.

In many experimental applications, $f(t)$ is not measured directly. Instead, the integral of $f(t)$ over an interval in t is observed. [Consider the example where $f(t)$ represents the count-rate function of some detection system. The total count recorded during any time interval is then the integral of $f(t)$ over that interval.] In such applications, where $f(t)$ does not change sign, it is appropriate to employ the law of the mean in a different way. One may write

$$I_i = \cos(\omega \bar{t}_i) \cdot F_i, \qquad \text{where} \quad F_i = \int_{t_i}^{t_{i+1}} f(t)\, dt. \tag{5}$$

Here $\bar{t}_i$ again represents some value of t in (t_i, t_{i+1}), and F_i is an experimental datum. If the set of experimental data $\{F_i\}$ does not cover the entire range of t, then gaps must be filled in by interpolation.

B. *Asymptotic Region*

The asymptotic contribution, $J(\omega, t_m)$, depends essentially upon the behavior of $f(t)$. In this region, t_m is chosen large enough so that a simple asymptotic representation of $f(t)$ is valid for all $t \geqslant t_m$. If $f_{as}(t)$ denotes this asymptotic representation, then $J_{ap}(\omega, t)$, the approximate asymptotic contribution, is

$$J(\omega, t_m) \cong J_{ap}(\omega, t_m) = \int_{t_m}^{\infty} f_{as}(t) \cos(\omega t)\, dt, \qquad (t \geqslant t_m). \tag{6}$$

With t_m sufficiently large, $J_{ap}(\omega, t_m)$ can be evaluated by expansion in an asymptotic series (i.e., in terms of inverse powers of t_m), giving to nth order

$$J_{ap}(\omega, t_m) = \sum_{k=1}^{n} \frac{a_k(\omega, t_m)}{t_m{}^k}. \tag{7}$$

It is usually necessary to retain only a few terms. The coefficients $\{a_k\}$ often contain sine and cosine terms, so that by propitious choice of t_m the leading-term coefficient a_1 can be made to vanish.

There exists another series expansion which may be useful between the near and asymptotic regions. Let $\{t_\nu\}$ represent the zeros of $\cos\{\omega t)$ in this intermediate region. Then the intermediate-region contribution, $K(\omega, t_0)$, is

$$K(\omega, t_0) = \sum_{\nu=1}^{N} A_{2\nu+1}, \qquad \text{where} \quad A_{2\nu+1} = \int_{t_{2\nu}}^{t_{2\nu+2}} f(t)\cos(\omega t)\, dt. \tag{8}$$

Using the Taylor-series expansion of $f(t)$ about $t = t_{2\nu+1}$ in Eq. (8), one finds

$$A_{2\nu+1} = \mp(1/\omega) \sum_{n=0}^{\infty} \frac{f^{(2n+1)}(t_{2\nu+1})}{(2n+1)!} (1/\omega)^{2n+1} \int_{-\pi}^{\pi} x^{2n+1} \sin x\, dx, \tag{9}$$

where the $(-)$ or $(+)$ sign applies if the principal value of $(\omega t_{2\nu+1})$ is $\frac{1}{2}\pi$ or $\frac{3}{2}\pi$, respectively. One finds for the first few terms

$$A_{2\nu+1} = \mp(1/\omega) \Big[(2\pi/\omega) f^{(1)}(t_{2\nu+1}) + \frac{\pi(\pi^2-6)}{3\omega^3} f^{(3)}(t_{2\nu+1}) + \frac{\pi(\pi^4 - 20\pi^2 + 120)}{60\omega^5} f^{(5)}(t_{2\nu+1}) + \cdots\Big]. \tag{10}$$

For $f(t)$ slowly varying compared to $\cos(\omega t)$, the higher-order terms will decrease quite rapidly. This expansion may be useful in the asymptotic region. Here, calculations should be carried out until $K(\omega, t_0) = J_{\mathrm{ap}}(\omega, t_0)$ is independent of N.

Accuracy can be estimated using the fact that $\Phi(\omega)$ should be independent of t_m, provided the asymptotic expansions are valid. Moreover, since t_m can be chosen sufficiently large, one can always satisfy the condition, $|I| \gg |J_{\mathrm{ap}}|$. Hence, the asymptotic term can be used to estimate that value of t_m for which I approximates $\Phi(\omega)$ to a specified degree of accuracy. The asymptotic term can also provide an estimate for the remainder of the infinite alternating series considered by Hurwitz and Zweifel [3]. One need no longer be concerned with the convergence properties of such series, because the calculation in the near region can be terminated as soon as a desired accuracy has been attained. This procedure can be quite effective in many applications where comparison with experiment requires a knowledge of Fourier transforms to only a few percent.

C. *Example*

Numerical results have been obtained for the Fourier integral [5]

$$\Phi(\omega) = \frac{2e^{-\alpha}}{\pi} \int_0^{\infty} \cos[(\omega-1)\,t]\, e^{-\beta^2 t^2} \exp\{\alpha e^{-\beta^2 t^2}\cos t\} \cos\{\alpha e^{-\beta^2 t^2} \sin t\}\, dt, \tag{11}$$

where α and β are parameters. For the near-region contribution, Eq. (4) was used. The asymptotic contribution for this case is to third order

$$J_{\text{ap}}(\omega, t_m) = -(-1)^n \left[\frac{2e^{-\alpha}}{\pi}\right] \frac{(\omega - 1)\exp(-\beta^2 t_m^{\,2})}{(4\beta^4 t_m^{\,2})}, \tag{12}$$

for values of t_m which satisfy $(\omega - 1)\, t_m = (n + \frac{1}{2})\,\pi$, with n an integer. Figure 1, which displays the resulting Fourier transform obtained for the parameter values

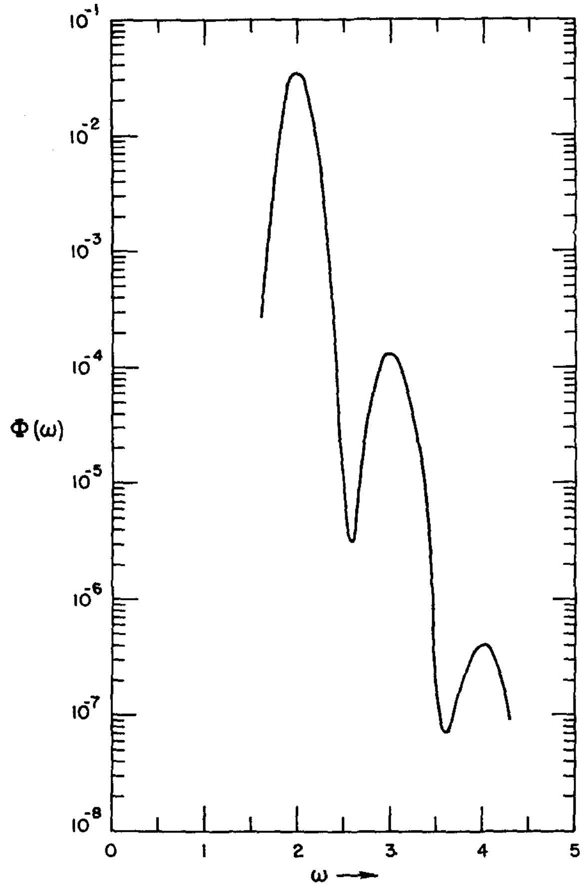

FIG. 1. The Fourier transform of

$$f(t) = (2e^{-\alpha}/\pi)\exp(-\beta^2 t^2)\exp[\alpha\exp(-\beta^2 t^2)\cos t] \times \cos[\alpha\exp(-\beta^2 t^2)\sin t]$$

for $\alpha = 0.01$ and $\beta = 0.06$ in the region $\omega \geqslant 1.6$.

$\alpha = 0.01$ and $\beta = 0.06$, demonstrates the general utility of this method. Here a relative accuracy of better than 2% in the value of $\Phi(\omega)$ has been maintained over a domain of about six decades.

References

1. L. N. G. Filon, *Proc. Royal Soc. Edinburgh*, **49**, 38 (1928).
2. Y. L. Luke, *Proc. Cambridge Phil. Soc.* **50**, 269 (1954).
3. H. Hurwitz, Jr., and P. F. Zweifel, *MTAC* **10**, 140 (1956).
4. O. F. Hastrup, Suffield Tech. Note No. 121, Department of National Defense, Canada (1964)
5. R. Gold, *Rev. Sci. Instr.* **36**, 784 (1965).

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