ON HIGH PRECISION METHODS FOR COMPUTING INTEGRALS OF OSCILLATORY FUNCTIONS*

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Abstract. A short account of the most important methods for the evaluation of integrals of oscillatory functions and an unified approach for such a purpose are given.

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1. INTRODUCTION

In the Fourier analysis, e.g. in the application of Fourier series or the inversion of Fourier and Laplace transform, as well as in many problems in physics and engineering, integrals of strongly oscillatory functions are appeared. For example, such integrals can be: 1° The Fourier coefficients

$$C_k(f) = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos kx\,dx, \qquad S_k(f) = \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin kx\,dx, \tag{1.1}$$

where $k \in \mathbb{N}$; 2° Integrals over $(0, +\infty)$,

$$C(f;\omega) = \int_0^{+\infty} f(x)\cos\omega x\,dx, \qquad S(f;\omega) = \int_0^{+\infty} f(x)\sin\omega x\,dx,$$

where ω is a large positive parameter; 3° Integrals involving Bessel functions

$$I_\nu(f;\omega) = \int_0^{+\infty} e^{-x^2} J_\nu(\omega x) f(x^2) x^{\nu+1}\,dx, \quad \nu > -1, \tag{1.2}$$

where ω is a large positive parameter. This type of integrals appears in some problems of high energy nuclear physics (cf. [1–3]).

For such integrals over finite or infinite limits there are a large number of special approaches, because the standard methods of numerical integration (for instance, formulas of Newton-Cotes or Gaussian type) require too much computation work and cannot be successfully applied.

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In this paper we give a short account of the most important methods for the evaluation of integrals of oscillatory functions (Sections 2 and 3), and an unified approach for such a purpose in Section 4.

2. FILON'S RULE, GAUSSIAN FORMULAE AND INTEGRATION BETWEEN ZEROS

The earliest formulas for numerical integration of rapidly oscillatory function are based on the picewise approximation by the low degree polynomials of $f(x)$ on the integration interval. The resulting integrals over subintervals are then integrated exactly. A such method was obtained by Filon [4].

Consider the Fourier integral on the finite interval

$$I(f;\omega) = \int_a^b f(x)e^{i\omega x}\,dx$$

and divide that interval $[a,b]$ into $2N$ subintervals of equal length $h = (b-a)/(2N)$, so that $x_k = a + kh$, $k = 0,1,\dots,2N$. The Filon's construction of the formula is based upon a quadratic fit for $f(x)$ on every subinterval $[x_{2k-2}, x_{2k}]$, $k = 1,\dots,N$ (by interpolation at the mesh points). Thus,

$$f(x) \approx P_k(x) = P_k(x_{2k-1} + ht) = \phi_k(t), \qquad t \in [-1,1], \tag{2.1}$$

where $P_k \in \mathcal{P}_2$, $k = 1,\dots,N$, and $\mathcal{P}_m$ denotes the set of all algebraic polynomials of degree at most m. It is easy to get

$$\phi_k(t) = f_{2k-1} + \frac{1}{2}(f_{2k} - f_{2k-2})t + \frac{1}{2}(f_{2k} - 2f_{2k-1} + f_{2k-2})t^2,$$

where $f_r \equiv f(x_r)$, $r = 0,1,\dots,2N$. Using (2.1) we have

$$I(f;\omega) \approx \sum_{k=1}^{N} \int_{x_{2k-2}}^{x_{2k}} f(x)e^{i\omega x}\,dx = h\sum_{k=1}^{N} e^{i\omega x_{2k-1}} \int_{-1}^{1} \phi_k(t)e^{i\theta t}\,dt,$$

where $\theta = \omega h$. Since $\int_{-1}^{1} \phi_k(t)e^{i\theta t}\,dt = Af_{2k-2} + Bf_{2k-1} + Cf_{2k}$, where

$$A = \overline{C} = \frac{1}{2}\int_{-1}^{1} (t^2 - t)e^{i\theta t}\,dt, \qquad B = \int_{-1}^{1} (1-t^2)e^{i\theta t}\,dt,$$

i.e.,

$$A = \frac{(\theta^2 - 2)\sin\theta + 2\theta\cos\theta}{\theta^3} + i\frac{\theta\cos\theta - \sin\theta}{\theta^2}, \qquad B = \frac{4}{\theta^3}(\sin\theta - \theta\cos\theta),$$

we obtain

$$I(f;\omega) \approx h\Big\{ i\alpha\left(e^{i\omega a}f(a) - e^{i\omega b}f(b)\right) + \beta E_{2N} + \gamma E_{2N-1}\Big\},$$

with $\alpha = (\theta^2 + \theta\sin\theta\cos\theta - 2\sin^2\theta)/\theta^3$, $\beta = 2(\theta(1+\cos^2\theta) - \sin^2\theta)/\theta^3$, $\gamma = 4(\sin\theta - \theta\cos\theta)/\theta^3$, and

$$E_{2N} = {\sum_{k=0}^{N}}'' f(x_{2k})e^{i\omega x_{2k}}, \qquad E_{2N-1} = \sum_{k=1}^{N} f(x_{2k-1})e^{i\omega x_{2k-1}},$$

where the double prime indicates that both the first and last terms of the sum are taken with factor 1/2. The limit $\theta \to 0$ leads to the Simpson's rule. The error estimate was given by Håvie [5] and Ehrenmark [6].

Improvements of the previous technique have been done by Flinn [7], Luke [8], Buyst and Schotsmans [9], Tuck [10], Einarsson [11], Van de Vooren and Van Linde [12], etc. For example, Flinn [7] used fifth-degree polynomials in order to approximate $f(x)$ taking values of function and values of its derivative at the points x_{2k-2}, x_{2k-1}, and x_{2k}. Stetter [13] used the idea of approximating the transformed function by polynomials in $1/t$. Miklosko [14] proposed to use an interpolatory quadrature formula with the Chebyshev nodes.

The construction of Gaussian formulae for oscillatory weights has also been considered (cf. Gautschi [15], Piessens [16–18]). Defining nonnegative functions on $[-1, 1]$,

$$c_k(t) = \frac{1}{2}(1 + \cos k\pi t), \quad s_k(t) = \frac{1}{2}(1 + \sin k\pi t), \quad k = 0, 1, \dots ,$$

the Fourier coefficients (1.1) can be expressed in the form

$$C_k(f) = 2\int_{-1}^{1} f(\pi t) c_k(t)\, dt - \int_{-1}^{1} f(\pi t)\, dt$$

and

$$S_k(f) = 2\int_{-1}^{1} f(\pi t) s_k(t)\, dt - \int_{-1}^{1} f(\pi t)\, dt.$$

Now, the Gaussian formulae can be obtained for the first integrals on the right-hand side in these equalities. For $k = 1(1)12$ Gautschi [15] obtained n-point Gaussian formulas with 12 decimal digits when $n = 1(1)8$, $n = 16$, and $n = 32$. We mention, also, that for the interval $[0, +\infty)$ and the weight functions $w_1(t) = (1 + \cos t)(1 + t)^{-(2n-1+s)}$ and $w_2(t) = (1 + \sin t)(1 + t)^{-(2n-1+s)}$, $n = 1(1)10$, $s = 1.05(0.05)4$, the n-point formulas were constructed by Krilov and Kruglikova [19].

Quadrature formulas for the Fourier and the Bessel transforms

$$F(x) = \int_0^{+\infty} t^\mu f(t) e^{i\omega t}\, dt, \quad H_k(x) = \int_0^{+\infty} t^\mu f(t) H_\nu^{(k)}(\omega t)\, dt, \quad k = 1, 2,$$

where ω is a real parameter and $H_\nu^{(k)}(t)$, $k = 1, 2$, are the Hankel functions, were derived by Wong [20].

Other formulas are based on the integration between the zeros of $\cos mx$ or $\sin mx$ (cf. [21–25]). In general, if the zeros of the oscillatory part of the integrand are located in the points x_k, $k = 1, 2, \dots , m$, on the integration interval $[a, b]$, where $a \le x_1 < x_2 < \dots < x_m \le b$, then we can calculate the integral on each subinterval $[x_k, x_{k+1}]$ by an appropriate rule. A Lobatto rule is good for this purpose (see Davis and Rabinowitz [21, p. 121]) because of use the end points of the integration subintervals, where the integrand is zero, so that more accuracy can be obtained without additional computation.

There are also methods based on the Euler and other transformations to sum the integrals over the trigonometric period (cf. Longman [26], Hurwitz and Zweifel [27]).

3. METHOD OF BAKHVALOV AND VASIL'EVA

A most significant progress in the development of high precision methods for Fourier integrals was made by Bakhvalov and Vasil'eva [28]. In their method $f(x)$ was expanded as a truncated series of Legendre polynomials $P_k(x)$, which could be integrated exactly term by term using the following closed formula

$$\int_{-1}^{1} P_k(x)e^{i\omega x}\,dx = i^k\sqrt{\frac{2\pi}{\omega}}J_{k+1/2}(\omega),$$

where J_ν is the Bessel function of the order ν. Thus, if $f(x) \approx \sum_{k=0}^{n} c_k P_k(x)$, then

$$\int_{-1}^{1} f(x)e^{i\omega x}\,dx \approx \sqrt{\frac{\pi}{2\omega}}\int_{-1}^{1} f(x)\sum_{k=0}^{n}(2k+1)i^k J_{k+1/2}(\omega)P_k(x)\,dx.$$

An approximation by Chebyshev polynomials was considered by Piessens and Poleunis [29]. An extension of the Bakhvalov and Vasil'eva method to the weighted integral $\int_a^b w(x)f(x)e^{i\omega x}\,dx$ was given by Patterson [30]. Precisely, he considered the cases $w(x) = (1-x^2)^{\pm 1/2}$ on the finite interval $(-1,1)$, $w(x) = x^\alpha e^{-x}$ on $(0,+\infty)$, and the Hermite case $w(x) = e^{-x^2}$ on $(-\infty,+\infty)$.

In a similar way, Gabutti [2] considered an integral of the form

$$I_0(f;\omega) = \int_0^{+\infty} e^{-x^2} J_0(\omega x)f(x^2)x\,dx,$$

which is a special case of (1.2). An asymptotic behaviour of this integral was investigated by Frenzen and Wong [31]. They showed that $I_0(f;\omega)$ decays exponentially like $e^{-\gamma\omega^2}$, $\gamma > 0$, when $f(z)$ is an entire function subject to a suitable growth condition.

4. AN UNIFIED APPROACH

Let $d\lambda(x)$ be a nonnegative measure on $\mathbb{R}$ with finite or infinite support, for which the all moments $\mu_\nu = \int_{\mathbb{R}} x^\nu\,d\lambda(x)$ exist for every ν and $\mu_0 > 0$. Define the inner product $(\,\cdot\,,\,\cdot\,)$ by

$$(f,g) = \int_{\mathbb{R}} f(x)g(x)\,d\lambda(x), \qquad \|f\|^2 = (f,f).$$

Then, there exist the (monic) orthogonal polynomials $\pi_k(\,\cdot\,) = \pi_k(\,\cdot\,,d\lambda)$, $k = 0,1,\ldots,$ which satisfy the three-term recurrence relation

$$\pi_{k+1}(x) = (x-\alpha_k)\pi_k(x) - \beta_k\pi_{k-1}(x), \quad k = 0,1,\ldots\,,$$

where $\pi_0(x) = 1$, $\pi_{-1}(x) = 0$, and

$$\alpha_k = \frac{(x\pi_k,\pi_k)}{(\pi_k,\pi_k)}\,, \qquad \beta_k = \frac{(\pi_k,\pi_k)}{(\pi_{k-1},\pi_{k-1})}\,.$$

In some cases (e.g. in the case of classical orthogonal polynomials) we have analytical expressions for the coefficients α_k and β_k. In a general case there exist numerical procedures for constructing these coefficients (for example, the method of (modified) moments and the discretized Stieltjes procedure).

The n-point Gaussian quadrature formula

$$\int_{\mathbb{R}} g(x)d\lambda(x) = \sum_{\nu=1}^{n} \lambda_\nu^{(n)} g(\tau_\nu^{(n)}) + R_n(g) \tag{4.1}$$

has maximum algebraic degree of exactness $2n-1$, in the sense that $R_n(g) = 0$ for all $g \in \mathcal{P}_{2n-1}$. In formula (4.1), $\tau_\nu = \tau_\nu^{(n)}$ are the *Gauss nodes*, and $\lambda_\nu = \lambda_\nu^{(n)}$ the *Gauss weights* or *Christoffel numbers*. This formula is also known as Gauss-Christoffel quadrature formula. A nice survey on that was given by Gautschi [32].

The nodes τ_ν are the zeros of the n-th orthogonal polynomial $\pi_n(\,\cdot\,, d\lambda)$, and the weights λ_ν, which are all positive, can be also expressed in terms of the same orthogonal polynomials. Precisely, the nodes τ_ν are the eigenvalues of the n-th order Jacobi matrix

$$J_n(d\lambda) = \begin{bmatrix} \alpha_0 & \sqrt{\beta_1} & & & \mathrm{O} \\ \sqrt{\beta_1} & \alpha_1 & \sqrt{\beta_2} & & \\ & \sqrt{\beta_2} & \alpha_2 & \ddots & \\ & & \ddots & \ddots & \sqrt{\beta_{n-1}} \\ \mathrm{O} & & & \sqrt{\beta_{n-1}} & \alpha_{n-1} \end{bmatrix},$$

where α_ν and β_ν are the coefficients in three-term recurrence relation for the monic orthogonal polynomials $\pi_n(\cdot, d\lambda)$. The weights λ_ν are given by $\lambda_\nu = \beta_0 v_{\nu,1}^2$, $\nu = 1, \dots, n$, where $\beta_0 = \int_{\mathbb{R}} d\lambda(t)$ and $v_{\nu,1}$ is the first component of the normalized eigenvector $\boldsymbol{v}_\nu$ corresponding to the eigenvalue τ_ν (cf. Golub and Welsch [33], and Gautschi [34]),

$$J_n(d\lambda)\boldsymbol{v}_\nu = \tau_\nu \boldsymbol{v}_\nu, \qquad \boldsymbol{v}_\nu^T \boldsymbol{v}_\nu = 1, \qquad \nu = 1, \dots, n.$$

There are well-known and efficient algorithms, such as the QR algorithm with shifts, to compute eigenvalues and eigenvectors of symmetric tridiagonal matrices (cf. the routine GAUSS in the package ORTHPOL given by Gautschi [35]). There are many methods for estimating the remainder term $R_n(g)$ in (4.1). Error bounds in the class of analytic functions were investigated by Gautschi and Varga [36].

Consider now

$$C(f; \omega, d\lambda) = \int_{\mathbb{R}} f(x) K(\omega, x)\, d\lambda(x),$$

where $K(\omega, x)$ is an oscillatory kernel and $f(x)$ is the "nonoscillatory" part of the integrand. In order to calculate this integral we need a polynomial approximation of the kernel $K(\omega, x)$. Let $K_n(\omega, \cdot\,)$ be the best $L^2(d\lambda)$-approximation of $K(\omega, \cdot\,)$ in $\mathcal{P}_n$. Then, it can be expressed in terms of orthogonal polynomials $\pi_k(x)$,

$$K(\omega, x) \approx K_n(\omega, x) = \sum_{\nu=0}^{n} a_\nu \pi_\nu(x). \tag{4.2}$$

Theorem 4.1. *Let $f, K(\omega, \cdot\,) \in L^2(d\lambda)$ and let $r_n(\omega; x) = K(\omega; x) - K_n(\omega, x)$, where the approximation $K_n(\omega; x)$ is given by (4.2). If*

$$b_k = \frac{1}{\|\pi_k\|^2} \int_{\mathbb{R}} f(x)\pi_k(x)\, d\lambda(x), \qquad k \geq 0, \tag{4.3}$$

then

$$C(f; \omega, d\lambda) = \int_{\mathbb{R}} f(x)K(\omega, x)\, d\lambda(x) = \sum_{k=0}^{n} a_k b_k \|\pi_k\|^2 + E_n,$$

where $|E_n| \leq \|r_n\|\|f\|$.

Proof. Since $E_n = C(f; \omega, d\lambda) - \sum_{k=0}^{n} a_k b_k \|\pi_k\|^2$, we have

$$\begin{aligned} E_n &= \int_{\mathbb{R}} f(x)K(\omega, x)\, d\lambda(x) - \sum_{k=0}^{n} a_k \int_{\mathbb{R}} f(x)\pi_k(x)\, d\lambda(x) \\ &= \int_{\mathbb{R}} f(x)\Big(K(\omega, x) - K_n(\omega, x)\Big)\, d\lambda(x) = \int_{\mathbb{R}} f(x) r_n(x)\, d\lambda(x), \end{aligned}$$

i.e., $E_n = (f, r_n)$. Now, Cauchy inequality gives $|E_n| = |(f, r_n)| \leq \|f\|\|r_n\|$. □

The coefficients b_k are given by (4.3). In order to calculate them exactly (up to rounding errors), when $f \in \mathcal{P}_n$, we use the $(n+1)$-point Gaussian formula (4.1). Thus,

$$b_k = \frac{1}{\|\pi_k\|^2} \sum_{\nu=1}^{n+1} \lambda_\nu^{(n+1)} f(\tau_\nu^{(n+1)})\pi_k(\tau_\nu^{(n+1)}), \qquad k = 0, 1, \ldots, n.$$

Indeed, here we have that $\mathrm{dg}(f(x)\pi_k(x)) = \mathrm{dg}\, f(x) + \mathrm{dg}\, \pi_k(x) \leq n + n = 2n < 2n + 1 = 2(n+1) - 1$. Thus, $n+1$ is the minimal number of nodes in the Gauss-Christoffel quadrature formula (4.1) for calculating b_k. So, the approximate value of the given integral can be expressed in the form

$$C(f; \omega, d\lambda) \approx \sum_{k=0}^{n} a_k \sum_{\nu=1}^{n+1} \lambda_\nu^{(n+1)} f(\tau_\nu^{(n+1)})\pi_k(\tau_\nu^{(n+1)}). \tag{4.4}$$

In many cases we know analytically the coefficients a_k in an expansion of $K(\omega; x)$. Now, we give some of such examples.

In [37, p. 560] we used that

$$\int_{-1}^{1} C_k^\lambda(x) e^{i\omega x}(1 - x^2)^{\lambda - 1/2}\, dx = i^k \frac{2\pi\Gamma(2\lambda + k)}{k!\Gamma(\lambda)(2\omega)^\lambda}\, J_{k+\lambda}(\omega), \quad \mathrm{Re}\, \lambda > -1/2,$$

where $C_k^\lambda(x)$ is the Gegenbauer polynomial of degree k. Taking this exact value of the integral we can find the following expansion of $e^{i\omega x}$ in terms of Gegenbauer polynomials,

$$e^{i\omega x} \sim \Big(\frac{2}{\omega}\Big)^\lambda \Gamma(\lambda) \sum_{k=0}^{+\infty} i^k (k + \lambda) J_{k+\lambda}(\omega) C_k^\lambda(x), \qquad x \in [-1, 1],$$

so that (4.4) becomes

$$C(f;\omega;d\lambda)\approx\Big(\frac{2}{\omega}\Big)^{\lambda}\Gamma(\lambda)\sum_{k=0}^{n} i^k(k+\lambda)J_{k+\lambda}(\omega)\sum_{\nu=1}^{n+1}\lambda_\nu^{(n+1)}f(\tau_\nu^{(n+1)})C_k^\lambda(\tau_\nu^{(n+1)}),$$

where $d\lambda(x)=(1-x^2)^{\lambda-1/2}\,dx$ on $(-1,1)$, and $\tau_\nu^{(n+1)}$ and $\lambda_\nu^{(n+1)}$, $\nu=1,\dots,n+1$, are nodes and weights of the $(n+1)$-point Gauss-Gegenbauer quadrature formula.

In some special cases we get: (1) For $\lambda=1/2$ – the method of Bakhvalov-Vasil'eva [28]; (2) For $\lambda=0$ and $\lambda=1$ – the method of Patterson [30].

Taking the expansion

$$e^{i\omega x}\sim e^{-(\omega/2)^2}\sum_{k=0}^{+\infty} i^k\frac{(\omega/2)^k}{k!}\,H_k(x),\qquad |x|<+\infty,$$

where H_k is the Hermite polynomial of degree n, we can calculate integrals of the form $\int_{-\infty}^{+\infty}e^{-x^2}e^{i\omega x}f(x)\,dx$. In a similar way we can use the expansion

$$e^{i\omega x^2}\sim\sum_{k=0}^{+\infty}\frac{(i\omega)^k}{k!2^{2k}(1-i\omega)^{k+1/2}}\,H_{2k}(x),\qquad |x|<+\infty.$$

Consider now the integral $I_\nu(f;\omega)$ given by (1.2)., which can be reduces to the following form

$$I_\nu(f;\omega)=\frac{1}{2}\int_0^{+\infty}e^{-t}J_\nu(\omega\sqrt{t})f(t)t^{\nu/2}\,dt=\frac{1}{2}\int_0^{+\infty}t^\nu e^{-t}\Big[t^{-\nu/2}J_\nu(\omega\sqrt{t})\Big]\,f(t)t^{\nu/2}\,dt,$$

where we put the oscillatory kernel in the brackets. Using the monic generalized Laguerre polynomials $\hat{L}_n^\nu(t)$, which are orthogonal on $(0,+\infty)$ with respect to the weight $t^\nu e^{-t}$, we get the expansion

$$t^{-\nu/2}J_\nu(\omega\sqrt{t})\sim\Big(\frac{\omega}{2}\Big)^{\nu}e^{-(\omega/2)^2}\sum_{k=0}^{+\infty}\frac{(-1)^k(\omega/2)^{2k}}{k!\Gamma(k+\nu+1)}\,\hat{L}_n^\nu(t),$$

so that

$$I_\nu(f;\omega)\approx\frac{1}{2}\Big(\frac{\omega}{2}\Big)^{\nu}e^{-(\omega/2)^2}\sum_{k=0}^{n}(-1)^k b_k\Big(\frac{\omega}{2}\Big)^{2k},$$

where b_k are the coefficients in the expansion of $f(t)$ in terms of $\hat{L}_n^\nu(t)$. In 1979 Gabutti [2] investigated in details the case $\nu=0$. Using a special procedure in D-arithmetic on an IBM 360/75 computer he illustrated the method taking an example with $f(t)=\sin t$ and $\omega=20$.

At the end we mention that it is possible to find exactly $I_\nu(f;\omega)$ when $f(t)=e^{i\alpha t}$. Namely,

$$I_\nu\big(e^{i\alpha t};\omega\big)=\frac{1}{2}\Big(\frac{\omega}{2}\Big)^{\nu}\frac{1}{(1-i\alpha)^{\nu+1}}\exp\Big[-\frac{(\omega/2)^2}{1-i\alpha}\Big].$$

The imaginary part of this gives the previous example of Gabutti [2].

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