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# Note

## Integration of Highly Oscillatory Functions

In this paper, we discuss the integration of highly oscillatory functions using (i) a new quadrature formula for evaluating integrals between two successive zeros of the integrand, and (ii) the iterated Aitken method for accelerating convergence in the case of an infinite interval when the integrand has an infinite number of zeros.

### 1. Introduction

The numerical integration of highly oscillatory functions $f(x)$ on $\mathbb{R}$ is a problem which frequently occurs in mathematical physics. Few papers[1] have been devoted to this question, except for integrals of the form $If = \int_0^\infty f(x)\, e^{ivx}\, dx$ [1–5].

We consider the integral $If = \int_a^b f(x)\, dx$ of a function $f \in C^{2n+2}(a, b)$, with a finite but large number of zeros on the bounded interval $(a, b)$ and with an infinite number of zeros in the case of an unbounded domain. The method of computation requires three steps.

(a) determination of the roots of $f(x)$ on $(a, b)$,

(b) computation of the integrals $I^i f = \int_{x_i}^{x_{i+1}} f(x)\, dx$ between two successive zeros,

(c) the third step is used only for an infinite interval $(a, b)$ in order to accelerate the convergence of the series $\sum_{i=1}^{\infty} I^i f$. The most original contribution of this paper is in the second step where $I^i f$, is computed with a Gauss–Jacobi formula giving for the same number of points more precise results than the usual Gauss–Legendre formula. We first consider the case of a bounded interval.

### 2. Integration of a Highly Oscillatory Function on a Bounded Interval

#### 2.1. *Determination of the Roots of the Integrand*

Finding the roots of $f(x) = 0$ on $(a, b)$ is not a difficult problem, assuming that all the roots are simple. It is sufficient to divide $(a, b)$ into subintervals of equal length $h \ll \frac{b-a}{s}$ and to locate a root in each subinterval using the Newton–Raphson method. If, for this particular value of $h$, only $r$ among the $s$ roots $x_i$ have been found, it is only necessary to start again with the function $f_1(x) = f(x)/\prod_{i=1}^{r} (x - x_i)$, since the Newton–Raphson method requires

$$\frac{f_1'(x)}{f_1(x)} = \frac{f'(x)}{f(x)} - \sum_{i=1}^{r} \frac{1}{x - x_i}.$$

[1] A noticeable exception is [9, 10].





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However, good results can often be obtained without calculating all of the roots of $f(x)$ on $(a, b)$.

### 2.2. *Computation of $I^i f$*

Let $\{x_i\}$ be the roots of $f(x)$ on $(a, b)$ and $I^i f = \int_{x_i}^{x_{i+1}} f(x)\, dx$,

$$I^i f = (x_{i+1} - x_i) \int_0^1 f[x_i + t(x_{i+1} - x_i)]\, dt, \qquad f(x) \in C^{2n+2}(x_i, x_{i+1}). \tag{1}$$

We first consider the following integral where $g(x)$ may have roots on (0, 1).

$$Jg = \int_0^1 x(1 - x)\, g(x)\, dx, \qquad g(x) \in C^{2n}(0, 1). \tag{2}$$

It is known [6] that an approximation $J_d g$ of degree $d = 2n - 1$ (that is exact for all polynomials of degree $d \leqslant 2n - 1$) of $J_g$ is

$$J_d g = \sum_{\alpha=1}^{n} W_{\alpha,n}\, g(t_{\alpha,n}), \tag{2'}$$

where $t_{\alpha,n}$ is a root of the Jacobi polynomial $H_n(x)$ such that

$$\int_0^1 x(1 - x)\, H_n(x)\, H_m(x)\, dx = \delta_{nm},$$

$\delta_{nm}$ being the Kronecker symbol. It is also well known that the Jacobi polynomial of degree $n$ has $n$ distinct real zeros contained in the interval (0, 1). We have [7]

$$H_n(x) = N_n x^{-1}(1 - x)^{-1} \frac{d^n}{dx^n} [x^{n+1}(1 - x)^{n+1}], \quad N_n = [(n + 1)(n + 2)(2n + 3)]^{1/2}$$

The weights $W_{\alpha,n}$ in (2′) are the Christoffel numbers defined by the relation

$$W_{\alpha,n} = 1 \Big/ \sum_{\nu=0}^{n-1} (H_\nu(t_{\alpha,n}))^2.$$

Let us now come back to $I^i f$; if we put $p(x) = x(1 - x)$, then comparison between (1) and (2) shows that (2′) leads to the following approximation $I_d^i f$ of $I^i f$.

$$I_d^i f = (x_{i+1} - x_i) \sum_{\alpha=1}^{n} \bar{\omega}_{\alpha,n} f[x_i + t_{\alpha,n}(x_{i+1} - x_i)], \qquad \bar{\omega}_{\alpha,n} = W_{\alpha,n} p^{-1}(t_{\alpha,n}), \tag{1'}$$

but from (2′) and from the definition of $p(x)$, it follows that in (1′), $d = 2n + 1$ instead of $d = 2n - 1$ for the Gauss–Legendre formula for the same number of points.

We wrote a program for computing $t_{\alpha,n}$, $W_{\alpha,n}$, $\bar{\omega}_{\alpha,n}$, $\alpha = 1, 2, \ldots, n$, $n \leqslant n_{\max} = 20$ but $t_{\alpha,n}$, $W_{\alpha,n}$ can be found in [8].

To be complete, we still have to compute, with the same degree $d = 2n + 1$ of approximation the two following integrals when $f(a) \neq 0$ and (or) $f(b) \neq 0$.

$$I^0 f = \int_a^{x_1} f(x)\, dx, \qquad I^s f = \int_{x_s}^{b} f(x)\, dx.$$

It is easy to prove that, if $x_i$ is not a zero of $f(x)$, then instead of (1′) we have

$$I_d^i f = (x_{i+1} - x_i)\left[K_0 f(x_i) + \sum_{\alpha=1}^{n} \bar{\omega}_{\alpha,n} f[x_i + t_{\alpha,n}(x_{i+1} - x_i)]\right],$$
$$K_0 = \tfrac{1}{2}\left(1 - \sum_{\alpha=1}^{n} \bar{\omega}_{\alpha,n}\right). \tag{1''}$$

Of course, there exists a similar expression with $K_0 f(x_{i+1})$ if $f(x_{i+1}) \neq 0$. The value of $K_0$ is obtained by computing the integral of a constant function on (0, 1).

Collecting all these results, the approximation $I_d f$ of degree $d = 2n + 1$ of $If$ is

$$I_d f = K_0[(x_1 - a) f(a) + (b - x_s) f(b)] + \sum_{\alpha=1}^{n} \bar{\omega}_{\alpha,n} \sum_{i=0}^{s} (x_{i+1} - x_i) f[x_i + t_{\alpha,n}(x_{i+1} - x_i)], \tag{3}$$

where, in the last summation, we put $x_0 = a$, $x_{s+1} = b$.

### 2.3. *Some Simple Formulas*

In some cases, quadrature formula (3) can lead to very lengthy computations and we consider here some different formulas with still good precision (but more difficult to estimate).

The first possibility is based on the two following remarks.

(1) In (2), as noted before, where $g(x)$ may have roots on (0, 1).

(2) The definition of the polynomials $H_n(x)$ implies that the roots $t_{\alpha,n}$ occur in pairs symmetric with respect to the point $x = \frac{1}{2}$ and from (2), (2′) the symmetric pairs have the same weight $W_{\alpha,n}$ and also the same modified weight $\bar{\omega}_{\alpha,n}$ since $p(x)$ is invariant under the transformation $x \to 1 - x$. As a consequence, if $g(x) = g(1 - x)$, then $I_d g - J_g = 0$ and formula (2′) is exact.

This suggests halving of the work by using the subintervals $(x_i, x_{i+2})$ instead of $(x_i, x_{i+1})$, and this gives, assuming that $S$ is an even number,

$$I_d f = K_0[(x_1 - a) f(a) + (b - x_s) f(b)] + \sum_{i>0}^{s/2} (x_{2i+2} - x_{2i}) f[x_{2i} + t_{\alpha,n}(x_{2i+2} - x_{2i})]. \tag{4}$$

It is trivial to write the corresponding expression for an odd number $S$. This approximation shows that valid results can be computed using only a subset of $\{x_i\}$.

An interesting approach, when $f(x)$ is not a smooth function, is to divide every interval $(x_i, x_{i+1})$ into $l$ equal subintervals applying in each of these $l$ subintervals a very simple formula with only one or two points. For instance, using only one point, since $t_{j,1} = \frac{1}{2}$ and $\bar{\omega}_{1,1} = \frac{2}{3}$, we have for $I^i f$ with $\lambda = (x_{i+1} - x_i)\, l^{-1}$,

$$I^i f = \frac{(x_{i+1} - x_i)}{3\lambda} \left\{ \sum_{j=1}^{l-1} f(x_i + j\lambda) + 2 \sum_{j=1}^{l} f[x_i + (j - \tfrac{1}{2})\lambda] \right\}. \tag{5}$$

Of course, one can use a mixture of (4) and (5).

## 3. Integration of a Highly Oscillatory Function on an Infinite Interval

Let us first assume that the series $\sum_{i=0}^{\infty} I^i f$ is convergent to $If$. Since $\sum_{i=0}^{\infty} I^i f$ is an alternating series, one knows at once the maximum error made by using the partial sum $S_m = \sum_{i=0}^{m} I^i f$. If, for $\epsilon$ given, $m$ is not too large, that is, if the series $\sum_{i=0}^{\infty} I^i f$ converges rapidly, we are, like in the case of a bounded interval,

(i) to look for the first (in an increasing order) $k$ zeros,

(ii) to compute $I^i f$ using the quadrature formulas (1′), (1″), or perhaps (4), (5).

Then relation (3) gives the approximation $I_{d,\epsilon} f$ of $If$.

If the series $\sum_{i=0}^{\infty} I^i f$ does not converge rapidly enough to obtain a practical value of $m$ for a given error $\epsilon$, we have to use some accelerating tools. We made a thorough numerical study of the $\epsilon$-algorithm, Euler's method, Padé approximants, and the iterated Aitken method. We experimentally found that this last method was the best suited to this particular problem and the reason why was discussed by the first author [11].

The iterated Aitken method is as follows: Let $\{S_m\}$ be the sequence of the partial sums $S_m = \sum_{i=0}^{m} I^i f$; then the sequence $\{T_{m,k}\}$ obtained after $k$ iterations of the Aitken method is defined by the relations

$$T_{m,0} = S_m, \qquad T_{m,k+1} = \frac{\Delta T_{m,k} T_{m+1,k} - \Delta T_{m+1,k} T_{m,k}}{\Delta T_{m,k} - \Delta T_{m+1,k}}, \qquad k, m = 0, 1, 2, \ldots,$$
$$\Delta T_{m,k} = T_{m+1,k} - T_{m,k}. \tag{6}$$

Broadly speaking, the iterated Aitken method runs succesfully as long as, for $k$ fixed, $\{T_{m,k}\}$ is an oscillatory sequence [11].

Notice that if the first $m$ partial sums $S_j$ are known, the maximum number of iterations is $K = [(m - 1)/2]$ (where $[(m - 1)/2]$ means the integer part of $(m - 1)/2$). From a practical point of view, in order to avoid a small denominator in (6) and since the convergence of the iterated Aitken method is very fast, the value of $K$ is 3 or 4, so $m$ is less than 10 (see Example 3).

We can even assume that the series $\sum_{0}^{\infty} I^i f$ does not converge and we conjecture the following result.

(i) if, for $K$ fixed, $K = 1, 2, 3, \ldots$, the sequences $\{T_{m,k}\}$ are oscillatory,

(ii) if $If$ exists in some sense,

then $T_{m,k}$ converges to $If$.

An example borrowed from [1] (the authors used the transformation due to Shanks, the simplest and most commonly used of these being equivalent to the iterated Aitken method) and discussed in the following section supports that conjecture.

## 4. Numerical Examples

In this section we give four examples to illustrate the previous theory. In all these examples,

(i) the integrals $I^i f$ between two successive zeros are computed with the quadrature formula (1′);

(ii) $h$ denotes the stepsize used to locate the zeros of the integrand while $n$ denotes the maximum number of points (roots of the Jacobi polynomials) used in the computation of $I^i f$;

(iii) The Newton–Raphson method was used to find the zeros of the integrand.

Example 1.

$$IJ^2 = \int_0^x J_p(\alpha t)\, J_p(\beta t)\, dt = (x/(\alpha^2 - \beta^2))[\beta J_{p-1}(\beta x)\, J_p(\alpha x) - \alpha J_{p-1}(\alpha x)\, J_p(\beta x)], \tag{7}$$

where $J_p(x)$ denotes the usual Bessel function.

(1) For $d = 2$, $\beta = 5$, $p = 3$, $x = 1$, with $h = 1/200$, $n = 10$, the quadrature formula (3) gave

$$I_d J^2 = 1.028299 \times 10^{-2}.$$

Exactly the same result is obtained with the right-hand side of (7).

(2) For $\alpha = 10$, $\beta = 20$, $p = 3$, $x = 1$, the following table gives for different values of $n$ the errors $\epsilon_1$, $\epsilon_2$, with

$$\epsilon = |\text{ exact value} - \text{computed value }| = |\ -2.154011972 \times 10^{-4} - \text{computed value }|.$$

When using respectively, the quadrature formulas (3) and (4).

| $n$ | $\epsilon_1$ | $\epsilon_2$ |
|---|---|---|
| 5 | $0.9 \times 10^{-7}$ | $0.2 \times 10^{-4}$ |
| 10 | $0.5 \times 10^{-13}$ | $0.25 \times 10^{-6}$ |
| 15 | $0.4 \times 10^{-13}$ | $0.1 \times 10^{-6}$ |
| 20 | $0.9 \times 10^{-14}$ | $0.7 \times 10^{-7}$ |

(3) For $\alpha = 20$, $\beta = 30$, $p = 2$, $x = 1$, the following table give the errors $\epsilon_1$, $\epsilon_2$, as in the previous case. The integrand has 14 zeros and the exact value of $IJ^2$ is $-9.327174830 \times 10^{-4}$.

| $n$ | $\epsilon_1$ | $\epsilon_2$ |
|---|---|---|
| 5 | $0.3 \times 10^{-7}$ | $0.6 \times 10^{-5}$ |
| 10 | $0.7 \times 10^{-8}$ | $0.15 \times 10^{-5}$ |
| 15 | $0.9 \times 10^{-9}$ | $0.7 \times 10^{-6}$ |
| 20 | $0.6 \times 10^{-9}$ | $0.4 \times 10^{-6}$ |

As a conclusion, theses results show that for the same number of function evaluations, it is better to use the quadrature formula (3) with $n$ than (4) with $2n$.

EXAMPLE 2.

$$IJ = \int_0^\infty x^{q-p} J_p(\alpha x)\, dx = 2^{q-p}\alpha^{p-q-1} \frac{\Gamma((q+1)/2)}{\Gamma(p - ((q-1)/2))}, \quad -1 < q < 2p + 1. \tag{8}$$

For $p = 3$, $q = 4$, $\alpha = 1$, the exact value is $IJ = 3$. Using the quadrature formula (3) with $n = 10$ and the iterated Aitken method (formula (6)) for $K = 3$ iterations, we obtained: $T_{j,3}\, J = 3.000022$.

EXAMPLE 3.

$$If = \int_0^\infty x^2 \sin 100x^2\, dx,$$

which converges in the Abel sense to $If = 3.1332853 \times 10^{-4}$.

We considered the iterated Aitken method for different values of $n$ and $k$ (the number of iterations); it appears that, probably due to roundoff errors, there exists for every $n$, an optimum $k_0$ so that for $k < k_0$, the error $\epsilon$ decreases regularly when $k$ increases, while, for $k > k_0$, $\epsilon$ has an erratic behavior. The following table gives the value of $k_0$ for some $n$.

| $n$ | $k_0$ | $\epsilon$ |
|---|---|---|
| 5 | 8 | $7 \cdot 10^{-9}$ |
| 10 | 6 | $3 \cdot 10^{-14}$ |
| 15 | 7 | $3 \cdot 10^{-14}$ |
| 20 | 8 | $5 \cdot 10^{-14}$ |

These results show and this conclusion has been strengthened by some other computations, that, from a practical point of view, the best value of $k$ is about 6 with $n$ between 5 and 10.

EXAMPLE 4. In this last set of examples, we consider integrals of the type $If = \int_0^{2\pi} f(x)\, e^{i\nu x}\, dx$. Of course, one can expect that the method of this paper is inferior to procedures which take the oscillatory nature of the integrand explicitly into account. To check this point, we made a comparison with some computations by Piessens and Poleunis [12], especially with respect to the Piessens–Gaussian rule (which is less effective than the other procedure described in [12]).

The following table concerning the integral $\int_0^{2\pi} x \cos x \sin mx \, dx$ (Table I) gives for some values of $m$ the errors $\epsilon$, in the first column according to [12], and in the other two columns according to the method described in this paper. In the second column, the number of function evaluations (number between brackets) is the same as for the Gauss rule while in the third column, $n$ is such that $\epsilon$ is almost the same. In both cases, the values of $n$ used in the computations are given.

TABLE I

Errors

| $m$ | Gauss rule [12] | This paper (1) | This paper (2) |
|---|---|---|---|
| 1 | $2 \cdot 10^{-15}$ (12) | $1 \cdot 10^{-15}$ (12) $n = 10$ | $1 \cdot 15^{-15}$ (12) $n = 10$ |
| 2 | $1 \cdot 10^{-15}$ (16) | $1 \cdot 10^{-10}$ (16) $n = 6$ | $1 \cdot 10^{-14}$ (24) $n = 10$ |
| 4 | $3 \cdot 10^{-15}$ (24) | $5 \cdot 10^{-7}$ (24) $n = 4$ | $2 \cdot 10^{-15}$ (40) $n = 8$ |
| 16 | $7 \cdot 10^{-15}$ (64) | $4 \cdot 10^{-3}$ (64) $n = 2$ | $2 \cdot 10^{-15}$ (144) $n = 7$ |
| 64 | $7 \cdot 10^{-16}$ (256) | $9 \cdot 15^{-4}$ (256) $n = 2$ | $3 \cdot 10^{-16}$ (1576) $n = 7$ |
| 256 | $2 \cdot 10^{-13}$ (512) | | $7 \cdot 10^{-12}$ (1792) $n = 5$ |

The two following tables (Tables IIA and B), concerning the integrals

$$I_1 = \int_0^{2\pi} \frac{x}{(1 - x^2/4\pi^2)^{1/2}} \sin mx \, dx, \qquad I_2 = \int_0^{2\pi} \log x \sin mx \, dx,$$

give the errors $\epsilon$ for the Piessens–Gauss rule and for the present method with $n = 10$.

TABLE IIA

Errors in $I_1$

| $m$ | Gauss rule [12] | This paper $n = 10$ |
|---|---|---|
| 1 | $1 \cdot 10^{-2}$ (18) | $1.5 \cdot 10^{-2}$ (20) |
| 2 | $5 \cdot 10^{-3}$ (36) | $1 \cdot 10^{-3}$ (40) |
| 4 | $4 \cdot 10^{-3}$ (72) | $8 \cdot 10^{-3}$ (80) |
| 10 | $3 \cdot 10^{-3}$ (186) | $5 \cdot 10^{-3}$ (200) |
| 20 | $2 \cdot 10^{-3}$ (360) | $3 \cdot 10^{-3}$ (400) |
| 30 | $2 \cdot 10^{-3}$ (540) | $2 \cdot 10^{-3}$ (600) |

TABLE IIB

Errors in $I_2$

| $m$ | Gauss rule [12] | This paper $n = 10$ |
|---|---|---|
| 1 | $1 \cdot 10^{-4}$ (18) | $3 \cdot 10^{-4}$ (20) |
| 2 | $8 \cdot 10^{-5}$ (36) | $1 \cdot 10^{-4}$ (40) |
| 4 | $4 \cdot 10^{-5}$ (72) | $6 \cdot 10^{-5}$ (80) |
| 10 | $1 \cdot 10^{-5}$ (180) | $3 \cdot 10^{-5}$ (260) |
| 20 | $7 \cdot 10^{-6}$ (360) | $1 \cdot 10^{-5}$ (400) |
| 30 | $5 \cdot 10^{-6}$ (540) | $1 \cdot 10^{-5}$ (600) |

As previously, the numbers between brackets give the number of function evaluations. For the last two integrals, results by both methods are similar. In conclusion, it appears that the present method is more useful for nontrigonometric applications.

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