Numerical Integrations in Maple and Mathematica

1. Not reliable for treating functions with singularities in higher dimensions.
2. They both rely on iterated integrals.

   Remark *For function* $f(x,y) = \frac{xy}{(x^2+y^2)^2}$ *if* $x^2+y^2 > 0$ *and* $f(x,y) = 0$ *if* $x^2+y^2 = 0$ *in the region* $[-1,1] \times [-1,1]$ *does not exist and yet the value of its repeated integrals is* 0*. Both Maple V Release 3 and Mathematica give the "wrong" answer* 0*.*

   $$\int_{-1}^{1}\int_{-1}^{1} f(x,y)dxdy$$

   It is strange that we can't evaulate this integral inside SWP with the Maple computation engine on, but the answer from Maple V, R3 is 0*. On the other hand, when we switch to Mathematica as a computation engine, we get the answer* 0*.*

3. Both Mathematica and Maple can't handle singularities which lie on the diagonal of a region.

Numerical integration and theoretical integration

1. Numerical integration experts can handle functions which are so called absolute integrals.
2. The non-absolute integrals, such as the following highly oscillatory function

   $$f(x,y) = \frac{\sin(\frac{1}{xy})}{xy},$$

   is not Lebesgue integrable but is Henstock integrable. Most experts in numerical integration do not talk about how to integrate this type of function directly. Most of the time, they recommend to use the transformation technique.
3. I and others (Lee, Peng Yee and his students) try to bridge the theorectical and numerical integrations.

Outline of the lecture

1. Use a non-uniform partition.
2. Closed Type Quadratures to take care of the absolute type of integrations.
3. Some experiments of the closed type quadratures.
4. Definition of Henstock integral.
5. Use the open type quadrature to estimate an example of the nonabsolute integral.
6. Singular points lie on a diagonal.
7. Error Bound and speed up of convergence (Romberg and Richardson schemes)

Closed type in one dimension (Ignore the

singularities)

First we experiment a closed type quadrature in one dimension, which can be used in estimating the integral of a monotone function with one singularity at one end point. A closed type quadrature is to ignore the singularity, see [DR]. We shall see that an adaptive quadrature in treating this type of function is more efficient than quadratures which use uniform spaced intervals. We therefore consider the following definition which enables us to divide an interval unevenly.

Uneven partition

Definition *A matrix A with positive* a_{nk} *is called uniformly regular if the following conditions are satisfied:*
(i) $\lim_{n\to\infty} a_{nk} = 0$ *uniformly over k.*
(ii) $\sum_{k=1}^{n} a_{nk} = 1.$

For example, we may use the finite sum formula, $\sum_{k=1}^{n} k^m,\ m = 1, 2, \ldots,$ to form uniform regular matrices. For $m = 1$, we define the matrix $a_{nk} = \frac{2k}{n(n+1)}$.

We remark that in Scientific Workplace, we may use

$$a(n,k) = \frac{2k}{n(n+1)}$$

In Maple, we may use

$$ank = (n,k) -> 2 * k/(n * (n+1));.$$

In Mathematica, we use

$$ank[n\_, k\_] := 2 * k/\{n * (n+1)\}.$$

(Which one is more natural to the users?) To illustrate what a uniform regular matrix would look like. We use Scientific Workplace to show the matrix determined by a_{nk} when $n = 10$, but first we modify $a(n,k)$ as follows:

$$a(n,k) = \begin{cases} \frac{2k}{n(n+1)} & if \quad k \leq n \\ 0 & if \quad k > n \end{cases}.$$

We obtain

$$\begin{matrix}
1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{3} & \frac{2}{3} & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{6} & \frac{1}{3} & \frac{1}{2} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{10} & \frac{1}{5} & \frac{3}{10} & \frac{2}{5} & 0 & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{15} & \frac{2}{15} & \frac{1}{5} & \frac{4}{15} & \frac{1}{3} & 0 & 0 & 0 & 0 & 0 \\
\frac{1}{21} & \frac{2}{21} & \frac{1}{7} & \frac{4}{21} & \frac{5}{21} & \frac{2}{7} & 0 & 0 & 0 & 0 \\
\frac{1}{28} & \frac{1}{14} & \frac{3}{28} & \frac{1}{7} & \frac{5}{28} & \frac{3}{14} & \frac{1}{4} & 0 & 0 & 0 \\
\frac{1}{36} & \frac{1}{18} & \frac{1}{12} & \frac{1}{9} & \frac{5}{36} & \frac{1}{6} & \frac{7}{36} & \frac{2}{9} & 0 & 0 \\
\frac{1}{45} & \frac{2}{45} & \frac{1}{15} & \frac{4}{45} & \frac{1}{9} & \frac{2}{15} & \frac{7}{45} & \frac{8}{45} & \frac{1}{5} & 0 \\
\frac{1}{55} & \frac{2}{55} & \frac{3}{55} & \frac{4}{55} & \frac{1}{11} & \frac{6}{55} & \frac{7}{55} & \frac{8}{55} & \frac{9}{55} & \frac{2}{11}
\end{matrix}$$

Consider the following closed type quadrature:

$$Q_n^1(f) = \frac{1}{2} a_{n1} f(u_{n1}) + \sum_{k=2}^{n} \frac{a_{nk}}{2} (f(u_{n,k-1}) + f(u_{nk})).$$

We would like to experiment this quadrature with the Scientific Workplace (which uses Maple as a tool for computation). But first we need to make the following adjustments for computation purpose. We define the right and left endpoints as follows:

$$\left[a(n,k) = \frac{2k}{n(n+1)} \right]$$

$$r(n,k) = \sum_{j=1}^{k} a(n,j)$$

and

$$l(n,k) = \sum_{j=0}^{k-1} a(n,j)$$

which correspond to $u_{n,k}$ and $u_{n,k-1}$ respectively.

We define our first closed type quadrature as follows:

$$Q_1(n) = (1/2)a(n,1)f(r(n,1)) + \sum_{k=2}^{n} \frac{a(n,k)}{2} (f(l(n,k)) + f(r(n,k)))$$

We note that the first term of $Q_1(n)$, $(1/2)a(n,1)f(r(n,1))$, is a tail term to take care of functions with a singularity, and the second term of $Q_1(n)$ is a trapezoidal sum. Thus, we may call the quadrature, $Q_1(n)$, to be the **adaptive trapezoidal sum**.

Example *Consider the function* $f(x) = \ln(1-\cos x)$*, if* $x \neq 0$*, and* $f(0) = 0$*. (We notice that* f *has a singularity at* $x = 0$*.) Use* $Q^1(n)$ *to approximate* $\int_0^1 \ln(1-\cos x)dx$*. If we use* ***Evaluate numerically*** *with Scientific Workplace under "Maple", we get the following numeric results:*

$$Q_1(300) = -2.720856531$$

$$Q_1(400) = -2.720938148$$

$$Q_1(430) = -2.720950937$$

We link with its Maple worksheet. We note that when we increase n, we will be warned of the existence of the singularity at $x = 0$*. To further investigate the convergence or divergence of this integral, we could write a separate program to run our quadrature.*

Remark *Consider the function* $f(x) = \frac{1}{\sqrt{1-x^2}}$*, if* $x \neq \pm 1$*, and* $f(0) = 0$*. We notice that* f *has a singularity at* $x = \pm 1$*, and* $\lim_{x\to -1^+} f(x) = +\infty$*, we use* $Q_1(n)$ *to approximate* $\int_{-1}^0 f(x)dx$ *(*1.57079633 *from Maple and Mathematica). Since our interval is not* $[0,1]$*, we need to modify the followings first*

$$\left[c(a,b,n,k) = \frac{2(b-a)k}{n(n+1)} \right]$$

$$r(a,b,n,k) = -1 + \sum_{j=1}^{k} c(a,b,n,j)$$

and

$$l(a,b,n,k) = -1 + \sum_{j=0}^{k-1} c(a,b,n,j)$$

$$Q_1(a,b,n) = (1/2)c(a,b,n,1)f(r(a,b,n,1)) + \sum_{k=2}^{n} \frac{c(a,b,n,k)}{2}(f(l(a,b,n,k)) + f(r(a,b,n,k)))$$

$$Q_1(-1,0,300) = 1.5666646$$

$$Q_1(-1,0,400) = 1.56769693$$

$$Q_1(-1,0,500) = 1.56831653$$

$$Q_1(-1,0,700) = 1.56902481$$

$$Q_1(-1,0,1000) = 1.56955614$$

$$Q_1(-1,0,1200) = 1.5697628$$

$$Q_1(-1,0,1400) = 1.56991042$$

$$Q_1(-1,0,1800) = ?$$

Let's investigate the results by using different uniform regular matrix:

$$d(a,b,n,k) = \frac{6(b-a)k^2}{n(n+1)(2n+1)}$$

$$r(a,b,n,k) = -1 + \sum_{j=1}^{k} d(a,b,n,j)$$

and

$$l(a,b,n,k) = -1 + \sum_{j=0}^{k-1} d(a,b,n,j)$$

$Q_1(a,b,n) = (1/2)d(a,b,n,1)f(r(a,b,n,1)) + \sum_{k=2}^{n} \frac{d(a,b,n,k)}{2}(f(l(a,b,n,k)) + f(r(a,b,n,k)))$

We obtain the following data:

$$Q_1(-1,0,300) = 1.57081229$$

$$Q_1(-1,0,400) = 1.57080895$$

$$Q_1(-1,0,500) = 1.57080645$$

$$Q_1(-1,0,700) = 1.57080331$$

$$Q_1(-1,0,1000) = 1.57080088$$

$$Q_1(-1,0,1200) = 1.57079994$$

$$Q_1(-1,0,1400) = 1.57079929$$

$$Q_1(-1,0,1800) = ?$$

We note that for this function f, the convergence is much faster (compared with the answer obtained from Maple or Mathematica) if we use the second order uniform regular matrix, $d(n,k)$.

Uniformly Regular Matrix is crucial.

We shall see that using $h = \frac{1}{2^k}$ alone won't work. Consider $c(n,k) = \frac{2^n}{2^k(2^n-1)}$, and note that $\sum_{k=1}^{n} c(n,k) = 1$. We define

$$r(n,k) = \sum_{j=1}^{k} c(n,j),$$

$$l(n,k) = \sum_{j=0}^{k-1} c(n,j),$$

We define our corresponding closed type quadrature as follows:

$$Q_2(n) = (1/2)c(n,1)f(r(n,1)) + \sum_{k=2}^{n} \frac{c(n,k)}{2}(f(l(n,k)) + f(r(n,k)))$$

$$Q_2(100) = -.787774556$$

Note that this is not even close to what we expected.

The tail term, $\frac{a(n,1)f(r(n,1)}{2}$, speed up the

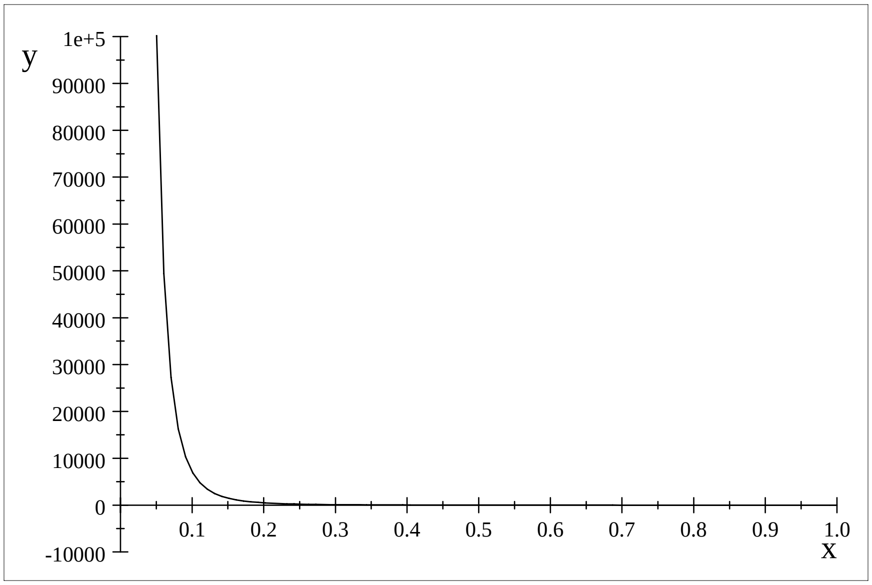
divergence

The next example shows that the tail term, $(1/2)a(n,1)f(r(n,1))$, could speed up the divergence too.

Example *Let* $f(x) = \frac{(\ln(1+x))^{1/7}}{x^4}$ *if* $x \neq 0$, *and* $f(0) = 0$. *We would like to use* $Q_1(n)$ *to approximate* $\int_0^1 f(x)dx \approx -2.72106545$. *The table below is a comparison between the quadrature with and without a tail.*

	without the tail $\frac{1}{2}a_{n1}f(u_{n1})$	with the tail $\frac{1}{2}a_{n1}f(u_{n1})$
$n = 100$	$0.3963290351 \times 10^{11}$	$0.1265245186 \times 10^{17}$
$n = 150$	$0.3982843325 \times 10^{12}$	$0.4030436606 \times 10^{18}$
$n = 200$	$0.2051511485 \times 10^{13}$	$0.4711286825 \times 10^{19}$

We conjecture from the table above that $\int_0^1 \frac{(\ln(1+x))^{1/7}}{x^4}dx = \infty$. We include the graph of f as follows: $\frac{(\ln(1+x))^{1/7}}{x^4}$



We now describe the error bound of this quadrature. The following two theorems can be found in [Y].

Theorem *Let* f *be improper Riemann integrable on* $(0,1]$, f'' *exist over* $(0,1)$ *and* a_{nk} *be a uniformly regular matrix. If the quadrature* $Q_n^1(f)$ *is used on* f *over the interval* $[0,1]$. *Then we have*

$$|E_n^1(f)| = \left|\int_0^1 f - Q_n^1(f)\right| \le \left|\int_0^{u_{n1}} f - u_{n1}f(u_{n1})\right| + \left|\frac{1}{2}a_{n1}f(u_{n1})\right| + \left|\sum_{k=2}^{n} -\frac{f''(c_{nk})a_{nk}^3}{12}\right|.$$

In view of Example 3 and Theorem 4, for a monotone function with singularity at one end point, to speed up the rate of convergence or divergence, we add an additional tail term, $\frac{1}{2}a_{n1}f(u_{n1})$ in $Q_n^1(f)$, or $(1/2)a(n,1)f(r(n,1))$ in $Q_1(n)$.

Derivative type tail correction

We may modify the tail term, $\frac{1}{2}a_{n1}f(u_{n1})$ in $Q_n^1(f)$, and, thus, introduce a second quadrature. In essence, it is to replace the tail, $\frac{1}{2}a_{n1}f(u_{n1})$, by a derivative term, $a_{n1}f(u_{n1}) - \frac{1}{2}a_{n1}^2 f'(u_{n1})$, which is obtained by considering the area of the trapezoid formed by tangent line at $x = u_{n1}$, x-axis and y-axis. Hence, if we set

$$Q_n^3(f) = a_{n1}f(u_{n1}) - \frac{1}{2}a_{n1}^2 f'(u_{n1}) + \sum_{k=2}^{n} \frac{a_{nk}}{2}(f(u_{n,k-1}) + f(u_{nk})).$$

We obtain the following information with the help of Maple V Release 3 Quadrature

$$Q_{300}^3(f) = -2.721138187$$
$$Q_{400}^3(f) = -2.721091402$$
$$Q_{430}^3(f) = -2.721081466.$$

Again, we can't increase the number n, but we can write a separate program to run this quadrature and we conjecture that the integral is convergent. Similar to $Q_n^1(f)$, we have the following

Theorem *Let f be improper Riemann integrable on* $(0,1]$, f'' *exist over* $(0,1)$ *and* a_{nk} *be a uniformly regular matrix. If the quadrature (8) is used on f over the interval* $[0,1]$. *Then we have*

$$|E_n^3(f)| = \left|\int_0^1 f - Q_n^1(f)\right| \le \left|\int_0^{u_{n1}} f - u_{n1}f(u_{n1})\right| + |u_{n1}f(u_{n1})| + \left|\frac{1}{2}a_{n1}^2 f'(u_{n1})\right| + \left|\sum_{k=2}^{n} -\frac{f''(c_{nk})a_{nk}^3}{12}\right|.$$

Remark *It is interesting to see that for* $f(x) = 1/\sqrt{x}$, *if* $x \ne 0$, *and* $f(0) = 0$, *if we use* $a_{nk} = \frac{2k}{n(n+1)}$, *then using* $Q_n^3(f)$ *is better than using* $Q_n^1(f)$, *meaning that* $Q_n^3(f)$ *uses less number of points for calculation and yet obtain desired accuracy. However, if we use* $b_{nk} = \frac{6k^2}{n(n+1)(2n+1)}$, *then* $Q_n^1(f)$ *is better than* $Q_n^3(f)$. *We illustrate these by observing the following data*

a_{nk}	b_{nk}
$Q_{80}^{1} = 1.973737918$	$Q_{80}^{1} = 1.999305311$
$Q_{80}^{3} = 1.991306127$	$Q_{80}^{3} = 2.001703454$
$Q_{90}^{1} = 1.976647478$	$Q_{90}^{1} = 1.999442063$
$Q_{90}^{3} = 1.992274385$	$Q_{90}^{3} = 2.001453908$

.

Further working on the derivative type tail correction

What we shall do next is to replace the tail, $(1/2)a(n,1)f(r(n,1))$, in $Q_1(n)$, by some additional terms.

1. We subdivide the interval $[0, a(n,1)]$ into n subintervals with the length $\frac{2^{-n}}{a(n,1)}$. for each subinterval (from the right to the left, i.e. the rightmost subinterval of $[0, a(n,1)]$ is with length $\frac{2^{-n}}{a(n,1)}$.) The reason we use the length of $\frac{2^{-n}}{a(n,1)}$ is hoping that we can use extrapolation to find the error bound for the tail term.
2. We apply the trapezoidal rule on the interval $[c(n,1), a(n,1)]$, and the derivative type on $[0, c(n,1)]$.
3. For each fixed n. Let's consider two intervals $I_1^n = [0, c(n,1)] \smile [c(n,1), a(n,1)]$ and $I_2^n = [a(n,1), 1]$. According to the quadrature above, we should be able to use the extrapolation method to find the error bound between I_1^n and I_1^{n+1} (i.e. we find the desired error bound on I_1 by increasing n). If the total errors (errors from I_1^n and I_2^n) do not get the desired error bound, then we come back and increase n and consider the new I_1^n, and I_2^n.

Accordingly, we consider the following defintions:

$$c(n,k) = \frac{2^n a(n,1)}{2^k(2^n - 1)}$$

$$L(n,k) = \sum_{j=0}^{k-1} c(n,j)$$

$$R(n,k) = \sum_{j=1}^{k} c(n,j)$$

$$Q_4(n) = c(n,1)f(R(n,1)) - \frac{1}{2}c^2(n,1)f'(R(n,1)) + \sum_{k=2}^{n} \frac{c(n,k)}{2}(f(L(n,k)) + f(R(n,k))) + \sum_{k=2}^{n} \frac{a(n,k)}{2}(f(l(n,$$

$$Q_4(300) = -2.72112033$$

$$Q_4(310) = -2.7211113$$

$$Q_4(315) = -2.72110771$$

Note that we obtain $\begin{cases} \int_0^1 \ln(1-\cos x) = -2.72106545 \text{ from Maple.} \\ \int_0^1 \ln(1-\cos x) = -2.72106545 \text{ from Mathematica.} \end{cases}$

Open type in two dimensions

Before we extend the closed type quadrature to two dimensions, we consider an open type quadrature in two dimensions by using two uniformly regular matrices, c_{nk}, d_{ml}, and denote them by $c(n,k)$ and $d(m,l)$ for computation purpose. Now set $c(n,k) = \frac{6k^2}{n(n+1)(2n+1)}$, $d(m,l) = \frac{6l^2}{m(m+1)(2m+1)}$, and consider the function $g(x,y) = \frac{1}{\sqrt{xy}}$ if $x \neq 0$, and $y \neq 0$, and $g(x,y) = 0$ if $x = y = 0$. First, we define the followings:

$$a(n,k) = \frac{6k^2}{n(n+1)(2n+1)}, r(n,k) = \sum_{j=1}^{k} a(n,j), l(n,k) = \sum_{j=0}^{k-1} a(n,j).$$

Next we define the following open quadrature:

$$Q(m,n) = \sum_{l=2}^{m}(\sum_{k=2}^{n} \frac{c(n,k)d(m,l)}{4}(g(r(n,k),r(m,l)) + g(l(n,k),r(m,l)) + g(r(m,l),l(n,k)) + g(l(n,k),l(m,l))))$$

We obtain the following information:

$$Q(20,20) = 3.94397632$$
$$Q(30,30) = 3.97226585$$
$$Q(40,40) = 3.98311667$$

We note that the quadrature should converge to 4. This experiment was orginated from Maple.

Remark *The open type quadrature is so called "avoiding the singularity" see [DR], and can be also used in estimating the integrals of functions which are highly oscillatory, such as* $f(x) = \frac{1}{x}\sin\frac{1}{x}$ *and* $f(x,y) = \frac{1}{xy}\sin\frac{1}{xy}$, *for details, see [LY].*

Remark *We briefly describe the process of approximating* $\int_0^1 \frac{1}{x}\sin\frac{1}{x}dx$ *(directly) without using the transformation technique. First we select a sequence* $\{x_i\}$ *with* $x_i = 5^{-(i-1)}$ *for* $i = 1,2,\ldots$ *, and apply the following closed type trapezoidal quadrature to approximate the integral of f in each* $I_i = [x_{i+1}, x_i]$, *denoted by* A_i.

$$Q_n(f) = \sum_{k=1}^{n} \frac{a_{nk}}{2}(f(u_{n,k-1}) + f(u_{nk}))$$

in which $u_{n0} = x_{i+1}$, *and* $u_{nk} = x_{i+1} + \sum_{p=1}^{k} a_{np}(x_i - x_{i+1})$. *Hence the estimate of integral of f over* $[0,1]$ *is given by the sum,* $\sum_{i=1}^{r} A_i$. *We remark that the quadrature is only a trapezoidal sum such that the weights and the abscissas are determined by a uniformly regular matrix,* a_{nk}.

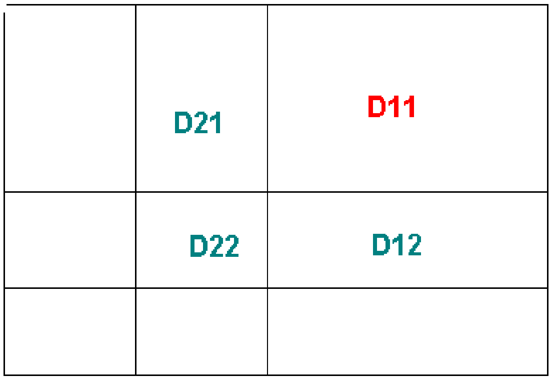
A nonabsolute integral

$$\int\int_{[0,1]^2} \frac{1}{xy} \sin \frac{1}{xy} .$$

Definition *A real-valued function f defined on a fixed interval in the* $n-$ *dimensional interval* E *is said to be Henstock integrable with the integral value* $F(E)$ *if for every given* $\epsilon > 0$ *there is a positive function* $\delta(x)$ *such that for every* $\delta-$*fine division* $D = \{(I,x)\}$ *of* E *we have*

$$\left|(D)\sum f(x)|I| - F(E)\right| < \epsilon.$$

1. Partition $[0,1] \times [0,1]$ as follows



2. Apply the open type quadrature on each D_{ij} and sum up the integrals.

Closed type in two dimensions

To speed up the rate of convergence for this type of function, naturally, we consider a closed type quadrature, which is an extension of $Q_n^1(f)$, as follows:

$$\begin{aligned} Q_n^5(f) = \sum_{l=2}^{m}\sum_{k=2}^{n} \frac{a_{nk}b_{ml}}{4}(f(u_{n,k-1},v_{m,l-1}) + f(u_{nk},v_{m,l-1}) + \\ f(u_{n,k-1},v_{ml}) + f(u_{nk},v_{ml})) \ + \frac{a_{n1}b_{m1}}{4}f(u_{n1},v_{m1}) \\ \sum_{k=2}^{n} \frac{a_{nk}b_{m1}}{4}(f(u_{n,k-1},v_{m1}) + f(u_{nk},v_{m1})) \ + \\ \sum_{l=2}^{m} \frac{a_{n1}b_{ml}}{4}(f(u_{n,1},v_{m,l-1}) + f(u_{n1},v_{ml})) \end{aligned}$$

If we use $a_{nk} = \frac{6k^2}{n(n+1)(2n+1)}$ and $b_{ml} = \frac{6l^2}{m(m+1)(2m+1)}$,we obtain the following information from Maple V Release 3:

$$\begin{aligned} Q_{70}^{5}(f) &= 3.999361277 \\ Q_{80}^{5}(f) &= 3.999619399 \\ Q_{90}^{5}(f) &= 3.999780084. \end{aligned}$$

By comparing the open type and closed type quadratures, we see that closed type quadrature is more efficient in this case.

Conclusion

1. Computer algebra systems are great tools for teaching and research. Users can use them to explore mathematics, making conjectures, verifying conjectures, and consequently formulating exciting new theorems.
2. CAS enables us to narrow the gap between the pure and applied mathematics.

DR (**bibitem**) Davis and Rabinowitz, method of Numerical Integration, 2nd ed., Academic Press 1983.

LY (**bibitem**) P.Y. Lee and W.-C. Yang, Henstock Integral and Numerical Integration, preprint.

Y (**bibitem**) W.-C. Yang, The Errors for the Closed and Open Type Adapted Quadratures, preprint.