Adaptive Quadratures, Henstock Integral, and Richardson and Romberg Methods

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Numerical integration

It is known that the highly oscillatory function such as $f(x,y) = \frac{\sin(\frac{1}{xy})}{xy}$ is not Lebesgue integrable and yet is Henstock integrable; the family of Lebesgue integrable functions is a subset of the family of Henstock integral functions. It is only meaningful to approximate a numerical integral when one can prove the existence of the integral. The algorithms of numerical integrations in higher dimensions used in many Computer Algebra Systems are not fully reliable. In this paper, we propose an adaptive quadrature, which uses non-even partitions, to handle integrands with singular points in higher dimensions, either highly oscillating or not. The quadrature is efficient when combined with Richardson or Romberg method on monotone functions.

Uniform regular matrices

We introduce a method of dividing an interval unevenly.

Definition. A matrix A with positive a_{nk} is called *uniformly regular* if the following conditions are satisfied:

1. $\lim_{n\to\infty} a_{nk} = 0$ uniformly over k.
2. $\sum_{k=1}^{n} a_{nk} = 1$.

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 $a_{nk} = \frac{2k}{n(n+1)}$. For example, a uniformly regular matrix looks like

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

For details, see [YC] and for a Maple code of generating a uniform regular matrix, click here.

Quadratures

Consider the following closed type quadrature

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

and the open type quadrature

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

where $u_{n,k} = \sum_{j=1}^{k} a_{n,j}$ and $u_{n,k-1} = \sum_{j=0}^{k-1} a_{n,j}$.

Note that the quadratures above can be called the **adaptive trapezoidal sum**. We shall use the combination of $Q_n^1(f)$ and $Q_n(f)$ to come up with the rule for **Richardson extrapolation integration** as follows

$$R_n(f) = \frac{1}{2}a_{n1}f(u_{n,1}) + \frac{1}{3}\left[4Q_n(f) - Q_{\frac{n}{2}}(f)\right]$$

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 $a_{n,k} = \frac{2k}{n(n+1)}$, we get the following numeric results from Maple:

$$Q_{300}^1(f) = -2.720856531$$
$$Q_{400}^1(f) = -2.720938148$$
$$Q_{430}^1(f) = -2.720950937$$

By using Maple V R4 on $R(n)$, we obtained the following info:

$$R_{300}(f) = -2.721249539$$
$$R_{400}(f) = -2.721164891$$
$$R_{430}(f) = -2.721149108$$

Notice that the **Richardson extrapolation** gives better estimate, the answer above is accurate up to 4 digits. However, we note that when we increase n, we will be warned of the existence of the singularity at $x = 0$ by Maple V R4. To further investigate the convergence of this integral, we could write a separate program to run our quadrature.

Open type in two dimensions

We mentioned an open type quadrature in two dimensions (see [YC]) by using two uniformly regular matrices, $c_{nk} = \frac{6k^2}{n(n+1)(2n+1)}$, and $d_{ml} = \frac{6l^2}{m(m+1)(2m+1)}$. Now consider the function

$$g(x,y) = \begin{cases} \frac{1}{\sqrt{xy}} & \text{if } x \neq 0, \text{ and } y \neq 0 \\ 0 & \text{if } x = y = 0 \end{cases}.$$

First, we define the followings: $u_{n,k} = \sum_{j=1}^{k} c_{n,j}, v_{n,k} = \sum_{j=1}^{k} d_{n,j}$.

Next we define the following open quadrature:

$$Q_{m.n}(g) = \sum_{l=2}^{m}\sum_{k=2}^{n} \frac{c_{nk}d_{ml}}{4}(g(u_{n,k-1}, v_{m,l-1}) + g(u_{nk}, v_{m,l-1}) + g(u_{n,k-1}, v_{ml}) + g(u_{nk}, v_{ml}))$$

We obtain the following information:

$$Q_{20,20}(g) = 3.94397632$$
$$Q_{30,30}(g) = 3.97226585$$
$$Q_{40,40}(g) = 3.98311667.$$

Now we use the two dimensional Richardson Extrapolation method:

$$R_n(g) = \frac{1}{3}\left[4Q_{n,n}(g) - Q_{\frac{n}{2},\frac{n}{2}}(g)\right].$$

We obtain the following data from Maple V R4: $R_{30}(g) = 3.993801507.$ Comparing with $Q_{30,30}(g) = 3.97226585,$ we see that the Richardson exploration speed up the convergence.

Closed type in two dimensions

We consider a closed type quadrature, which is an extension of $Q_n^1(f)$, as follows:

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

If we use $a_{nk} = \frac{6k^2}{n(n+1)(2n+1)}$ and $b_{ml} = \frac{6l^2}{m(m+1)(2m+1)}$ on the function g above, we obtain the following information from Maple V Release 4:

$$Q_{70}^2(g) = 3.999361277$$
$$Q_{80}^2(g) = 3.999619399$$
$$Q_{90}^2(g) = 3.999780084$$

By comparing the open type and closed type quadratures, we see that closed type quadrature is more efficient in this case. Moreover, we predict that the convergence will be improved if we incorporate the Richardson extrapolation with the closed type quardrature on this function.

Singularities lie on a diagonal line

Consider evaluating the following numerical integral

$$(1)\ \int_0^1\int_0^1 \cos 2\pi x \cos 2\pi y \begin{pmatrix} \log(x-y)^2 - \\ \log\left(1+(x-y)^2\right) \end{pmatrix} dxdy$$

Both Maple and Mathematica could not give an answer due the singularities lie along $x = y.$ What we will do is to transform the singularities to the boundary first and apply a quadrature which uses uniformly regular matrices for computations. Note that the function $f(x,y) = \cos 2\pi x \cos 2\pi y\left(\log(x-y)^2 - \log\left(1+(x-y)^2\right)\right)$ is symmetric with respect to $y = x,$ so we consider the integration over the triangle with vertices $O = (0,0),$ $P = (1,0)$ and $Q = (1,1).$ After the transformation with change of variables, $u = x,$ and $v = x - y,$ the singular points are shifted to x- axis, and the Jacobian is $\begin{vmatrix} u_x & u_y \\ v_x & v_y \end{vmatrix} = abs\begin{vmatrix} 1 & 0 \\ 1 & -1 \end{vmatrix} = 1.$ Thus, equation (1) becomes

$\int_0^1 \int_0^1 \cos 2\pi u \cos 2\pi(u-v)(\log v^2 - \log(1+v^2))dudv$. By using the uniformly regular matrices $a_{nk} = \frac{2(b-a)k}{n(n+1)}$, and $b_{ml} = \frac{2(b-a)l}{m(m+1)}$, and write a corresponding Pascal program, we obtain the following information

$$Q_{400,400}(f) = -.223374393133243$$
$$Q_{600,600}(f) = -.223411046499008$$
$$Q_{800,800}(f) = -.223421583469551$$
$$Q_{1000,1000}(f) = -.223425232050112$$

Richardson Extrapolation mentioned above will speed up the convergence, *but authors need to write a traditional program (based on this Richardson's method) to do further experiments.*

Remarks

1. We can predict that given a function with two variables, there should be an optimal choice for picking the uniform regular matrices, a_{nk}, and b_{nk}.
2. Richardson Extrapolation in two dimensions works well in speeding up the convergence.

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