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Numerical Integration of Functions with a Sharp Peak at or near One Boundary Using Möbius Transformations

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A class of coordinate transformations depending on a single parameter is studied as quadrature tool. Working rules for the choice of the parameter are proposed. Numerical tests for the method are presented. They show that these coordinate transformations, when combined with Gauss–Legendre quadrature rules, are well suited for the numerical integration of functions possessing a sharp peak *at or near* one boundary of the interval of integration. A method to combine the transformations with automatic quadrature routines is also proposed; it seems to be useful for the numerical evaluation of integrals with the same kind of integrand behavior. © 1990 Academic Press, Inc.

1. INTRODUCTION

Quite often in practice one encounters the problem of how to integrate functions with a sharp peak. In most cases such an integration can be done only numerically. Usually the position of the peak and/or its width are known at least roughly. For example, in our investigations concerning multicenter molecular integrals with exponential-type functions [1] we encountered integrals of the form

$$I = \int_0^1 w(s; m, n, \alpha, \beta, p) f(s, p)\, ds \tag{1.1}$$

with weight function ($p, \alpha, \beta \in \mathbb{R}_+$; $m, n \in \mathbb{N}$)

$$w(s; m, n, \alpha, \beta, p) = \frac{(1-s)^m s^n}{[p^2 s(1-s) + \alpha^2(1-s) + \beta^2 s]^{m+n+1/2}}. \tag{1.2}$$

Integral I is part of the integrand of an outer integral with integration variable p. The weight function (1.2) exhibits very sharp peaks for certain combinations of the parameters (m, n, α, β, p), especially for large p. A straightforward calculation

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shows that the location of the peaks may be obtained quite easily as zeroes of a third-order polynomial.

A number of quadrature methods turned out to be inappropriate in this situation, mainly because of the computational costs caused by the sharp peaks:

—Automatic routines [2] are accessible in software libraries [3, 4], but even sophisticated routines [5, 6] have some disadvantages [7, 8].

—For Gaussian rules [9], either the standard ones, or newly computed Gaussian rules [9] with respect to Eq. (1.2), also the numerical error estimation is difficult [10].

It is more cost effective to use all available information on the behavior of the integrand to make the integrand function smoother and to flatten its peaks. This can be done through coordinate transformations [11–16]. For example, the IMT-rule [17, 18] can be understood this way. Then many quadrature methods perform better for the new integrand.

In this paper we shall study a simple class of coordinate transformations: *Möbius transformations* [19, 20], also called *bilinear* or *fractional linear transformations*, depending on a single parameter. The additional numerical effort to implement it as a quadrature tool is (usually) negligible since no transcendental functions have to be computed. For the problem described above these transformations seem to be very effective. First results of the method concerning integrals with weight function (1.2) were presented at a conference.[1] Now, more generally, we shall see that these coordinate transformations are well suited for the quadrature of functions with a sharp peak at or near a boundary of the interval of integration.

In the following section we describe how to use these Möbius transformations in combination with Gauss–Legendre rules as quadrature tools. Classes of functions for which the method is exact will be given explicitly.

In the subsequent section we will report on the implementation and numerical tests of the method. Working rules for the choice of the parameter will be presented.

The results will be discussed and summarized in the last section. We will see that the use of Möbius transformations in combination with fixed quadrature rules or with automatic routines makes the numerical quadrature of functions with a sharp peak at or near a boundary much more efficient.

In an appendix an equivalent formulation of the method in terms of quadrature rules is presented. Here we study Möbius transformations in combination with *Gauss–Jacobi rules*: This allows us to point out a connection of our method to some well-known quadrature rules.

[1] Sanibel Symposium 1988 on Atomic, Molecular and Condensed Matter Theory, University of Florida, Whitney Marine Laboratory, St. Augustine, Florida, March 12–19, 1988.

2. Möbius Transformations as Quadrature Tools

In numerical quadrature coordinate transformations are used to obtain a more favorable integrand, and then a fixed quadrature rule or even an automatic routine is used to evaluate the transformed integral.

The result of using the coordinate transformation

$$x = \varphi(u) \tag{2.1}$$

with $a = \varphi(c)$, $b = \varphi(d)$ to obtain

$$I = \int_a^b f(x)\,dx = \int_c^d g(u)\,du \tag{2.2}$$

with the *new integrand*

$$g(u) = f(\varphi(u))\,\varphi'(u), \tag{2.3}$$

and applying a fixed quadrature rule G_n with weights w_j and abscissae u_j to the u-integral is

$$G_n(g) = \sum_{j=1}^{n} w_j\, g(u_j). \tag{2.4}$$

It may be formulated entirely in terms of the original integrand $f(x)$ as

$$G_n(g) = \sum_{j=1}^{n} w_j\, \varphi'(u_j)\, f(\varphi(u_j)) = R_n(f), \tag{2.5}$$

i.e., as a fixed quadrature rule R_n with abscissae $x_j = \varphi(u_j)$ and weights $\omega_j = w_j \varphi'(u_j)$.

Unless otherwise stated we will use the notation G_n for an n-point Gauss–Legendre rule in the sequel.

First we consider the case where $[a, b]$ and $[c, d]$ are bounded intervals. There is no loss of generality assuming $[a, b] = [c, d] = [-1, 1]$ since this can always be achieved by suitable linear coordinate transformations.

We study the one-parameter system of Möbius transformations

$$x = \varphi(\xi; u) = \frac{u + \xi}{1 + \xi u} \tag{2.6}$$

with inverse

$$u = \chi(\xi; x) = \frac{x - \xi}{1 - \xi x} \tag{2.7}$$

for $-1 < \xi < 1$. Here we regard ξ as a parameter, and u and x as independent variables. Hence φ' denotes the derivative of φ with respect to u in the following. Using (2.6) as coordinate transformation in combination with G_n yields exact results whenever $g(u)$ is a polynomial of degree less than $2n$, i.e., when $f(x)$ is of the form

$$f(x) = \frac{1}{(1-\xi x)^2} P_{2n-1}\left(\frac{x-\xi}{1-\xi x}\right) \tag{2.8a}$$

$$= \frac{1}{(1-\xi x)^2} \tilde{P}_{2n-1}\left(\frac{1}{1-\xi x}\right) \tag{2.8b}$$

$$= \sum_{j=2}^{2n+1} b_j \left(\frac{1}{1-\xi x}\right)^j, \tag{2.8c}$$

where $P_m(t)$ and $\tilde{P}_m(t)$ denote any—in general different—polynomials in t of degree less or equal to m, and b_j are arbitrary constants. This parallels to a certain extent the results of Newbery [11] on exponential and trigonometric polynomials.

Now we consider the case where $[a, b]$ is a semi-infinite interval. Without loss of generality we may assume $[a, b] = [0, \infty]$ and $[c, d] = [-1, 1]$. In this case we may use the Möbius transformation

$$x = \Phi(\xi; u) = \xi \frac{1+u}{1-u} \tag{2.9}$$

with inverse

$$u = X(\xi; x) = \frac{x-\xi}{x+\xi} \tag{2.10}$$

for $0 < \xi < \infty$ as coordinate transformation. Applying G_n to the new integrand gives exact results if $f(x)$ is of the form

$$f(x) = \frac{1}{(x+\xi)^2} P_{2n-1}\left(\frac{x-\xi}{x+\xi}\right) \tag{2.11a}$$

$$= \frac{1}{(x+\xi)^2} \tilde{P}_{2n-1}\left(\frac{1}{x+\xi}\right) \tag{2.11b}$$

$$= \sum_{j=2}^{2n+1} b_j \left(\frac{1}{x+\xi}\right)^j. \tag{2.11c}$$

In Appendix A it is shown how the quadrature method based on the coordinate transformations of both cases can be formulated in terms of quadrature rules. The case of the unbounded interval is seen to be completely equivalent to the Gauss–rational rules available in the NAG-library [21, 22]. Therefore no test results for this case will be given in the next section. It seems probable that the rules corresponding to the case of the bounded interval—or equivalently, the coordinate transformations (2.6)—will turn out to be of comparable practical importance in view of the test results presented in the following section.

3. Application and Numerical Tests

The numerical quadrature of a function with a sharp peak at or near a boundary of integration, which is based upon Möbius transformations, requires the choice of a certain ξ. First, we discuss how ξ should be chosen in order to utilize information on the position and/or the width of the peak. Second, we will compare our method to other quadrature rules by presenting numerical test values for various functions. These functions all have a sharp peak at or near a boundary of integration and may be taken as quite typical representatives. Further we will report on test results obtained for various choices of ξ. We will see that there is normally quite a large interval of ξ-values yielding acceptable results.

We consider the coordinate transformation (2.6) on $[-1, 1]$. If the original integrand peaks in $[x - \Delta x/2, x + \Delta x/2]$ then this interval is mapped to an u-interval of approximate length

$$\Delta u = [\varphi'(\xi; \chi(\xi; x))]^{-1} \Delta x. \tag{3.1}$$

Thus if $\varphi'(\xi; \chi(\xi; x))$ is small the peak region can be expanded enormously, and hence the new integrand poses less problems for numerical quadrature via G_n. Equivalently we may say that the abscissae of the new rule R_n obtained from G_n using (2.5) and (2.6) cluster in the region of the peak.

Since the extrema of $\varphi'(\xi; u)$ are

$$\varphi'(\xi; 1) = \frac{1-\xi}{1+\xi}, \qquad \varphi'(\xi; -1) = \frac{1+\xi}{1-\xi}, \tag{3.2}$$

i.e., directly at the boundaries, by continuity $\varphi'(\xi; u)$ is small for $u \approx \xi$, i.e., near one boundary, if $|\xi| \approx 1$.

These facts suggest the following two working rules which both assume $|\xi| \approx 1$:

Working Rule W. *If the function f has a sharp peak at one boundary and attains half of the peak value at or close to $x = x_0$, choose $\xi = x_0$ and use the corresponding Möbius transformation* (2.6).

If the function has a sharp peak near one boundary and attains half of its peak value at that $x = x_0$ which has the largest distance from the boundary (there may be two points inside the integration interval where the function attains half of its peak value!) then use the Möbius transformation (2.6) *with $\xi = x_0$.*

If the point x_0 is chosen as described above then the bulk of the peak is contained in one of the x-intervals $I_+ = [\xi, 1]$ or $I_- = [-1, \xi]$. That interval is expanded by a large factor by $\chi(\xi; x)$ to the corresponding u-interval, $J_+ = [0, 1]$ or $J_- = [-1, 0]$, resp., if $|\xi| \approx 1$.

This Working Rule W can be used if the width and the position of the peak are known. If only the position is known one may use the following working rule:

WORKING RULE W′. *If the function f has a sharp peak at or close to* $x = x_0$ *choose* $\xi = x_0$ *and use the corresponding Möbius transformation* (2.6).

First we consider the case that function f has its peak *exactly at* the boundary. Then Rule W′ is not applicable. Rule *W* has the effect of enlarging the half width at half maximum from approximately $1 - |\xi|$ for f to about 1 for the transformed function $h(u) = f(\varphi(\xi; u))$. The extra factor $\varphi'(\xi; u)$ of the new integrand $g(u)$ is large near the boundary opposite to the peak. Therefore extra weight is given to that interval, where the transformed function is supposed to be small. Ideally this can lead to a very broad peak of the new integrand near $u = 0$.

These effects are illustrated in Fig. 1. This plot shows the function

$$f(x) = \frac{250}{\pi} (1 + 2500(5x + 5)^2)^{-1}, \tag{3.3}$$

the transformed function $h(u)$, and the new integrand $g(u)$ for $\xi = -0.996$.

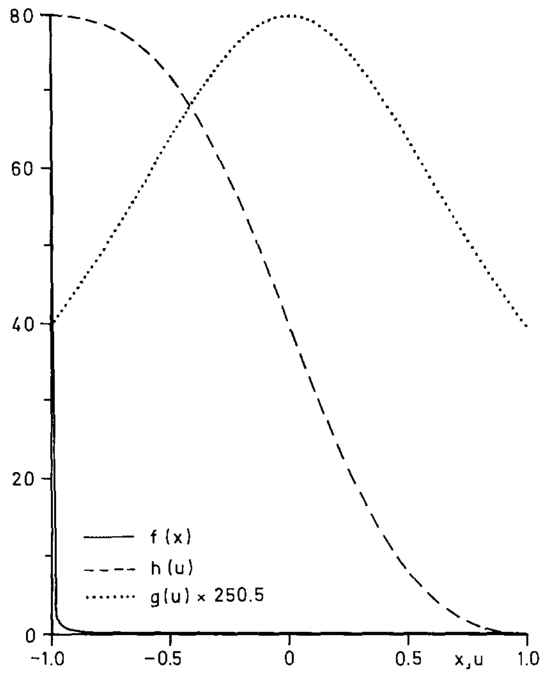

FIG. 1. Plotted are function $f(x)$ of (3.3), the transformed function $h(u)$ and the new integrand $g(u)$ corresponding to it for $\xi = -0.996$.

In the case that the function f has its peak *close* to one boundary both Working Rules W and W′ may be applied. The effect of Rule W′ is that the transformed function peaks at $u=0$. Rule W works as in the former case. In any case and by both working rules the width of the peak is increased enormously.

Now we report on numerical tests of the method. The computations were done in FORTRAN 77 DOUBLE PRECISION, corresponding to an accuracy of 14–15 decimal digits on our computer.

In Table I we present results for the following functions:

(a) The function (3.3) possessing a peak *at* one boundary.

(b) The function

$$f(x)=0.0199\,\frac{(x-0.99)^{24}}{(1-0.99x)^{26}}, \tag{3.4}$$

which is of the form (2.8). Apart from relative rounding errors of the order of $10^{14}\times n$, where n is the order of the Gauss–Legendre rule used, our transform method is indeed exact for $n>12$.

(c) The functions

$$f(x)=50\,\frac{(50x+50)^{10}}{[1+10(50x+50)^2]^{13/2}}, \tag{3.5a}$$

$$f(x)=\frac{21}{5e^{30x-30}+2e^{-(30x-30)}}, \tag{3.5b}$$

possessing a sharp peak *near* one boundary.

TABLE I

Comparison of the Method of the Present Article with Composite Gauss–Legendre Rules with m Subintervals for Various Functions on the Interval $[-1, 1]$

Function	ξ	Present method	Legendre rules $m=1$	Legendre rules $m=2$	Working rule
(3.3)	−0.996	7/14	74/173	148/346	W
(3.4)	0.99	12/13	183/***	44/92	—
(3.5a)	−0.9884	13/22	104/***	204/348	W
(3.5a)	−0.983	14/24	104/***	204/348	W′
(3.5b)	$0.89\bar{3}$	10/18	29/59	24/96	W
(3.5b)	$0.98\bar{3}$	19/39	29/59	54/96	W′

Note. In the case of the composite Legendre rule with $m=2$ the two intervals $[-1, \xi]$ and $[\xi, 1]$ are used. Plotted are the numbers n_5/n_{10} of functional evaluations needed to achieve 5- and 10-figure accuracy, resp. Three stars mean that the corresponding number is greater than 200. The ξ-value used in (2.6) and the corresponding working rule are indicated.

From Table I it is clear that Rule W is superior to Rule W′—if this rule is applicable. In fact, Rule W utilizes more information than does Rule W′. But it is seen that even application of Rule W′ leads to results superior to Gauss–Legendre rules.

Hence it is not optimal to think of the peak *position* alone: The whole peak *region* should be considered. This also explains why our method with highest resolution *at* one boundary, see (3.2), also gives good results for the functions (3.5). The method of the present article is not sensitive to the exact value of ξ; there is normally a large interval of ξ-values yielding acceptable results. This may be seen from Table II. In terms of quadrature rules one might say: It is important to have a sufficient number of abscissae in the peak region; then their exact positions—determined by the value of ξ—do not matter very much.

Thus we conclude that it is preferable to use Rule W if possible, since the corresponding ξ-value is closer to the optimal ξ-range than the value corresponding to rule W′.

TABLE II

Möbius Transformation (2.6) Combined with Gauss–Legendre Rule G_n Applied to the Integral of Function (3.5b) in the Interval $[-1, 1]$ with $n \in \{6, 12, 18, ..., 90\}$ for Different ξ

ξ \ n	6	12	18	24	30	$n(13)$
$0.98\bar{3}$	3	3	4	5	7	60
$0.96\bar{6}$	2	5	6	7	9	42
0.950	3	5	7	10	11	36
$0.93\bar{3}$	3	5	8	10	13	30
$0.92\bar{6}$	3	5	9	11	13	30
0.920	3	5	9	11	13	30
$0.91\bar{3}$	3	7	9	13	13	24
$0.90\bar{6}$	3	6	9	12	13	30
0.900	3	5	9	12	13	30
$0.89\bar{3}$	3	7	10	13	13	24
$0.88\bar{6}$	3	6	9	13	13	24
0.880	2	5	9	13	13	24
$0.87\bar{3}$	3	5	9	13	13	24
$0.86\bar{6}$	3	6	10	12	13	30
$0.85\bar{3}$	3	6	9	13	13	24
$0.83\bar{3}$	2	6	8	12	13	30
$0.76\bar{6}$	3	5	7	10	12	36
$0.66\bar{6}$	2	4	7	7	11	42
$0.33\bar{3}$	0	3	3	5	7	—
0.000	1	2	3	4	5	—

Note. Plotted is the number of exact decimal digits after rounding. $n(13)$ is the first value of n in the specified range where 13 exact digits are obtained. Gauss-Legendre rules correspond to $\xi = 0$. Working Rule W′ corresponds to $\xi = 0.98\bar{3}$, while the ξ-value corresponding to Rule W is close to $\xi = 0.89\bar{3}$.

Though our main emphasis in this paper is laid on fixed quadrature rules it may be noted that Möbius transformations can also be used together with automatic quadrature routines.

We chose the routine D01AJF of the NAG library as an all-purpose automatic integrator. The performance of the routine may be controlled by giving two input parameters EPSABS and EPSREL as user defined absolute and relative error requirements. The output is the value of the integral, the number of integrand evaluations, and an estimated absolute error of the result. We chose EPSABS = 0 always.

When D01AJF was applied to function (3.3) on $[-1, 1]$ the routine needed 357 integrand evaluations for EPSREL $= 10^{-9}$, and 399 evaluations for EPSREL $= 10^{-13}$. When D01AJF was applied to the new integrand $g(u)$ corresponding to function (3.2) for $\xi = -0.996$ (compare Fig. 1), only 63 integrand evaluations were needed for both relative error requirements. But it should be noted that the transform method based on Gauss–Legendre rules needs only 20 integrand evaluations in this case for the same accuracy: In all cases the observed error was less than 10^{-14}.

Thus if information on peak position or width is available it may be worth trying to combine automatic routines with the appropriate Möbius transformation. This approach seems to be efficient enough for normal users. It also may be extended easily to other coordinate transformations. A more complicated application of Möbius transformations is the development of special-purpose automatic integrators [23]. Which approach is better may be worth investigating by further numerical studies.

4. Discussion and Summary

Coordinate transformations in integrals allow the use of relevant information on the behavior of the integrand to obtain new integrands which are easier to integrate. Thus the numerical quadrature of functions with a sharp peak at or close to one boundary of the interval of integration may be performed more efficiently since the new integrand function is smoother and has a less pronounced peak.

In this paper we showed that Möbius transformations of a special type for finite intervals, Eq. (2.6), in combination with Gauss–Legendre rules or general-purpose automatic integrators are well suited for this purpose. It should be noted that the numerical effort to implement these coordinate transformations is low, since no additional transcendental functions have to be computed.

The coordinate transformation (2.6) depends on one parameter ξ which has to be chosen in some way: Information on the width and/or position of the peak should suffice for this choice. We suggested and tested two working rules, W and W′. It turned out that Rule W led to better results than Rule W′ in the examples studied. This is not surprising since essentially Rule W utilizes information *both* on peak position *and* width while Rule W′ relies only on knowledge of the position.

Certainly in each application of Möbius transformations as quadrature tools there will be a range of adequate ξ-values. In the examples studied, this range turned out to be broad; Working Rule W—and a bit less efficiently also rule W'—were useful to locate this range; the choice of ξ did not seem to be critical. It may be conjectured that this holds in general.

The main emphasis in this paper is laid on coordinate transformations combined with standard Gauss rules. This method considerably facilitates the numerical quadrature of certain classes of functions without the necessity of computing non-standard Gauss rules corresponding to special weight functions. In the case of Eq. (2.6) combined with Gauss–Legendre rules we were able to determine all those functions explicitly for which our method is exact. The results presented in Section 3 show that the quadrature method for bounded intervals presented in Section 2 are useful for the quadrature of functions with a sharp peak at or near one boundary of the interval of integration. Though we have tested the method only for a limited number of functions we think that we have chosen examples which are typical enough to justify the statement about its usefulness. For semi-infinite intervals the present method using Möbius transformations (2.9) in combination with Gauss–Jacobi rules is equivalent to the well-known Gauss–rational rules. This sheds new light upon rules obtained using Möbius transformations for the finite interval in combination with Gauss–Legendre rules: They can be viewed as rational rules as well.

In certain situations automatic integrators will be preferable to fixed rules. Fortunately it is possible to combine coordinate transformations with automatic routines as was described in the previous section. If an adequate transformation is chosen, one can make use of the reliability of automatic quadrature and largely avoid the costs of automatic integrators which are not adapted to the integrand. In this way it is not necessary to develop a special-purpose automatic integrator for every class of application. Instead, coordinate transformations are used as a tool which does not require too much highly specialized knowledge on how to program a good special-purpose automatic quadrature routine. In this paper we have shown how this problem can be solved for the quadrature of functions with a sharp peak at or close to one boundary of the interval of integration via Möbius transformations.

APPENDIX A: QUADRATURE RULES

We discuss how the transform method using the coordinate transformations (2.6) and (2.9) can be formulated in terms of quadrature rules.

In the case of bounded intervals one may use (2.6) in combination with $G_n = J_n^{(\alpha,\beta)}$, the n-point Gauss–Jacobi rule with abscissae u_j and weights w_j corresponding to the weight function $w^{(\alpha,\beta)}(u) = (1-u)^\alpha(1+u)^\beta$ on $-1 \leqslant u \leqslant 1$ for $\alpha > -1$, $\beta > -1$. With (2.5), we obtain new rules, $R_n = M_n^{(\alpha,\beta,\xi)}$, with abscissae

$x_j = \varphi(\xi; u_j)$ and weights $\omega_j = w_j \varphi'(\xi; u_j)$ depending on n, α, β, and ξ. These rules evaluate $I = \int_{-1}^{1} f(x)\,dx$ exactly, whenever $f(x)$ is of the form

$$f(x) = \frac{(1-x)^\alpha (1+x)^\beta}{(1-\xi x)^{\alpha+\beta+2}} P_{2n-1}\left(\frac{x-\xi}{1-\xi x}\right) = \frac{(1-x)^\alpha (1+x)^\beta}{(1-\xi x)^{\alpha+\beta+2}} \tilde{P}_{2n-1}\left(\frac{1}{1-\xi x}\right) \qquad \text{(A.1)}$$

for $\xi \neq 0$. Equation (A.1) holds because then the new integrand corresponding to f is a polynomial of degree not greater than $2n-1$, multiplied by $w^{(\alpha,\beta)}$. Equation (2.8) is the special case $\alpha = \beta = 0$ of (A.1) corresponding to the use of Gauss–Legendre rules. It is easy to show that these new rules converge to the exact value of the integral for all Riemann-integrable functions in the limit $n \to \infty$.

In the case of semi-infinite intervals one can also construct quadrature rules using (2.9) but we will see that these rules are well known. We use (2.9) in combination with $G_n = J_n^{(\alpha,\beta)}$ to obtain new rules $R_n f = \sum_{j=1}^{n} \omega_j f(x_j)$ with abscissae $x_j = \Phi(\xi; u_j)$ and weights $\omega_j = w_j \Phi'(\xi; u_j)$ depending on n, α, β, and ξ. These rules evaluate exactly $I = \int_0^\infty f(x)\,dx$, whenever both $\xi > 0$ holds, and $f(x)$ is of the form

$$f(x) = \frac{x^\beta}{(x+\xi)^{\alpha+\beta+2}} P_{2n-1}\left(\frac{x-\xi}{x+\xi}\right) = \frac{x^\beta}{(x+\xi)^{\alpha+\beta+2}} \tilde{P}_{2n-1}\left(\frac{1}{x+\xi}\right), \qquad \text{(A.2)}$$

since then the new integrand corresponding to f is a suitable polynomial multiplied by the Gauss–Jacobi weight function. But in the notation of Ref. [21] Gauss–rational rules

$$S = \sum_{i=1}^{n} w_i f(x_i), \qquad \text{(A.3)}$$

with adjusted weights w_i and abscissae x_i, exactly evaluate the integral $I = \int_a^\infty f(x)\,dx$ whenever

$$f(x) = \frac{|x-a|^c}{|x+b|^d} P_{2n-1}\left(\frac{1}{x+b}\right), \qquad \text{(A.4)}$$

where $c > -1$, $d > c+1$, $a+b > 0$, and $P_m(t)$ stands for any polynomial in t of degree m or less. Comparing with (A.2), we see that we have reproduced these rules for $a = 0$, $b = \xi$, $c = \beta$, $d = \alpha + \beta + 2$. This means that—up to a translation of the interval of integration—the use of Gauss–rational rules is equivalent to applying the coordinate transformation (2.9).

Hence we have established a relation between Gauss–rational rules on one hand and Möbius transformations for the semi-infinite interval combined with Gauss–Jacobi rules on the other hand. Thus one can view rules obtained from the Möbius transformation (2.6) using Gauss–Jacobi rules as G_n, as an adaptation of Gauss–rational rules to the case of a bounded interval.

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