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Integration Points for the Reduction of Boundary Conditions*

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An analysis of a method for the numerical evaluation of the integral $\int_a^b f(x)\,dx$ is presented. The method introduces a change of variable, $x = x(q)$, with the property that $d^n x/dq^n$ is zero at $x = a$, $x = b$ for $n = 0, 1, 2, \ldots N$, where N is an integer to be chosen. The Euler-Maclaurin formula shows that the resulting integral in the variable q is ideally suited for numerical integration, using equally spaced points and equal weights in q-space. Examples are given for various integrals which occur in quantum chemistry and applications to more than one dimension are discussed.

Key words: Numerical integration

For the numerical integration of many dimensional integrals a change of variable to make zero various low order derivatives at the boundaries has been variously used. [See Boys and Rajagopal (1965), Boys and Handy (1969) and a special scheme by Sag and Szekeres (1964), where a device which makes all boundary derivatives equal to zero is used. The latter is similar to the T_∞ transformation introduced below.] For an approximate estimate of the errors in transformations of such types, the most useful data appear to be the results for various one dimensional integrals. These do not appear to have been available and such a set is given here. Since these transformations are the simplest way of making various derivatives have zero values at the boundaries of the integration range, they will be referred to here as boundary derivative reductions.

The type of transformations with which we are concerned is the simplest type of change of variable $x(q)$ with

$$\int_0^1 F(x)\,dx = \int_0^1 F(x(q))\,\frac{dx}{dq}\,dq \equiv \int_0^1 G(q)\,dq\,. \qquad (1)$$

It is always arranged that dx/dq varies as q^a near $q = 0$ and $(1-q)^a$ near $q = 1$. Then the simplest numerical approximation to this with $n+1$ equally spaced

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points (including the two limits) is

$$\sum_{i=1}^{n-1} G(q_i \equiv i/n) + 0.5(G(0)+G(1))$$
$$= \int_0^1 F(x)\,dx - \frac{n^{-2}}{12}(G^{(1)}(1) - G^{(1)}(0)) + \frac{n^{-4}}{720}(G^{(3)}(1) - G^{(3)}(0)) \tag{2}$$
$$- \frac{n^{-6}}{30240}(G^{(5)}(1) - G^{(5)}(0)) + 0(n^{-8}).$$

The terms varying as n^{-2}, n^{-4} etc. are the correction terms given by the Euler-Maclaurin formula [see Krylov (1962) or Whittaker and Robinson (1937)]. But these depend on the values of the odd derivatives at the boundary. If $a+b>1$, where q^b denotes the variation of $F(x(q))$ for small q, then the n^{-2} term vanishes; if further $a+b>3$, then the n^{-4} term vanishes and so on. In the transformations T_3 and T_5 used below, we generally have residuals of n^{-4} and n^{-6} respectively. The integrals without transformation generally give n^{-2} errors and these are given for comparison.

It is considered that for the evaluation of many dimensional integrals, the use of such transformations for each dimension separately is probably the most desirable first step for most integrals. In such a case it is desirable to be able to estimate the value of the errors to be expected. Such errors for $n=6$ to about $n=12$ in the tables provide an approximate means of doing this and seem to be the only record of suitable quantities for this.

The notations T_p with p giving the lowest power of q are used in the tables for the following transformations with T_1 thus denoting no transformation:

$$T_1:\ x=q$$
$$T_2:\ x=a_2\int_0^1 q(1-q)\,dx = 3q^2-2q^3$$
$$T_p:\ x=a_p\int_0^1 q^{p-1}(1-q)^{p-1}\,dq \tag{3}$$
$$T_\infty:\ x=[\exp(-q^{-1})]\,[\exp(-q^{-1})+\exp(-(1-q)^{-1})]^{-1}.$$

The constants a_p are chosen to make x cover the range 0 to 1 as q covers the same range. The numerical integration for a given $F(x)$ is then performed through Eq. (1) and through

$$\left(\int_0^1 G(q)\,dq\right)_{\text{approximate}} = \sum_{i=1}^{n-1} G(i/n) + 0.5(G(0)+G(1)). \tag{4}$$

The fractional errors ε obtained by these transformations are given for different n, all multiplied by 10^5, so that 1. denotes a normal high accuracy. In each table a quantity (error $\times(n^p)$) is recorded as $(\,)_p$. This is the value of C if the error varied as Cn^{-p}. Hence the constancy of $(\,)_p$ in a column denotes a close approximation to an n^{-p} law. The fractional error results are stated to 0.00001 but there may be errors of about 0.00002 and so any case less than 0.00005 has been given as 0. The accurate standard of reference was taken from $n=100$, T_∞, and so this has no entry.

Table 1. Fractional errors $\times 10^5$ for $F = \exp(-4(x-0.5)^2)$

n	T_1		T_3		T_5		T_∞
6	−915.6	$(-0.3296)_2$	−38.46	$(-0.4985)_4$	311.4	$(145.3)_6$	−196.3
8	−514.2	$(-0.3291)_2$	−13.59	$(-0.5566)_4$	15.42	$(40.42)_6$	−116.7
10	−328.8	$(-0.3288)_2$	−5.368	$(-0.5368)_4$	1.345	$(13.45)_6$	−3.632
12	−228.3	$(-0.3287)_2$	−2.526	$(-0.5239)_4$	0.3356	$(10.02)_6$	12.10
16	−128.3	$(-0.3286)_2$	−0.7790	$(-0.5106)_4$	0.05830	$(9.781)_6$	0.5658
20	−82.13	$(-0.3285)_2$	−0.3151	$(-0.5042)_4$	0.01531	$(9.799)_6$	−0.4428
40	−20.52	$(-0.3284)_2$	−0.01938	$(-0.4962)_4$	0.00021	$(8.599)_6$	−0.00075
60	−9.122	$(-0.3284)_2$	−0.00383	$(-0.4965)_4$	0		0
100	−3.284	$(-0.3284)_2$	−0.00049	$(-0.4959)_4$	0		—

Table 2. Fractional errors $\times 10^5$ for $F = \exp(x-0.5)^2$

n	T_1		T_3		T_5		T_∞
6	543.6	$(0.1957)_2$	−85.06	$(-1.102)_4$	54.75	$(25.54)_6$	−853.5
8	306.2	$(0.1959)_2$	−27.74	$(-1.136)_4$	8.781	$(23.02)_6$	−271.7
10	196.1	$(0.1961)_2$	−11.51	$(-1.151)_4$	2.337	$(23.37)_6$	0.9609
12	136.2	$(0.1962)_2$	−5.589	$(-1.159)_4$	0.7845	$(23.42)_6$	28.65
16	76.66	$(0.1962)_2$	−1.781	$(-1.167)_4$	0.1399	$(23.48)_6$	1.304
20	49.07	$(0.1963)_2$	−0.7319	$(-1.171)_4$	0.03671	$(23.49)_6$	−1.046
40	12.27	$(0.1963)_2$	−0.04597	$(-1.177)_4$	0.00558	$(22.85)_6$	−0.00176
60	5.454	$(0.1963)_2$	−0.00909	$(-1.179)_4$	0		0
100	1.963	$(0.1963)_2$	−0.00117	$(-1.177)_4$	0		—

Table 3. Fractional errors $\times 10^5$ for $F = 0.5\cosh(2x-1)$

n	T_1		T_3		T_5		T_∞
6	942.2	$(0.3327)_2$	−91.61	$(-1.187)_4$	63.27	$(29.51)_6$	1014.2
8	520.3	$(0.3329)_2$	−30.33	$(-1.242)_4$	9.834	$(25.78)_6$	−301.3
10	333.1	$(0.3331)_2$	−12.67	$(-1.267)_4$	2.607	$(26.07)_6$	2.296
12	231.4	$(0.3332)_2$	−6.177	$(-1.281)_4$	0.8752	$(26.13)_6$	31.88
16	130.2	$(0.3332)_2$	−1.975	$(-1.294)_4$	0.1560	$(26.18)_6$	1.447
20	83.31	$(0.3333)_2$	−0.8133	$(-1.301)_4$	0.04093	$(26.20)_6$	−1.164
40	20.83	$(0.3333)_2$	−0.05119	$(-1.311)_4$	0.00625	$(25.61)_6$	−0.00196
60	9.259	$(0.3333)_2$	−0.01013	$(-1.314)_4$	0		0
100	3.333	$(0.3333)_2$	−0.00132	$(-1.315)_4$	0		—

The transformation T_∞ is a special form introduced because it has all the boundary derivatives zero. It can be inferred non-rigorously by inspection of the simple Euler-Maclaurin formula that the errors would decrease more rapidly than any finite power of n^{-1}. This can also be shown by more complicated vigorous mathematical argument. It will be seen that the results for T_∞ in every table appear to be in agreement with this.

The tables show how markedly improved are the results for T_3 and T_5 compared to T_1 in all normal cases (Tables 1–3) and how closely they follow Euler-Maclaurin predictions. A few exceptional functions are included and again

Table 4. Fractional errors $\times 10^5$ for $F = \sin(\pi x)$

n	T_1		T_2		T_3		T_∞
6	−2295.1	$(-0.8262)_2$	112.6	$(1.460)_4$	−21.31	$(-9.942)_6$	405.5
8	−1288.4	$(-0.8246)_2$	35.90	$(1.471)_4$	− 4.144	$(-10.86)_6$	−10.41
10	− 823.8	$(-0.8238)_2$	14.74	$(1.474)_4$	− 1.118	$(-11.18)_6$	− 8.088
12	− 571.8	$(-0.8234)_2$	7.121	$(1.476)_4$	− 0.3803	$(-11.35)_6$	0.2640
16	− 321.4	$(-0.8230)_2$	2.256	$(1.478)_4$	− 0.06873	$(-11.53)_6$	0.04567
20	− 205.7	$(-0.8228)_2$	0.9244	$(1.479)_4$	− 0.01815	$(-11.62)_6$	− 0.01048
40	− 51.40	$(-0.8225)_2$	0.05779	$(1.480)_4$	− 0.00030	$(-12.54)_6$	0
60	− 22.84	$(-0.8225)_2$	0.01141	$(1.478)_4$	0		0
100	− 8.224	$(-0.8225)_2$	0.00148	$(1.481)_4$	0		—

Table 5. Fractional errors $\times 10^5$ for $F = \exp(-100(x-0.5)^2)$

n	T_1		T_3		T_5	T_∞
6	5727.5	$(2.016)_2$	76371.1	$(989.8)_4$	131406.8	88076.3
8	361.2	$(2.312)_2$	33717.0	$(1381.0)_4$	73641.6	41723.3
10	10.34	$(0.1034)_2$	12746.7	$(1274.6)_4$	39857.7	17265.9
12	0.1344	$(0.0002)_2$	4038.0	$(837.3)_4$	19857.7	6006.6
16	0		246.7	$(161.6)_4$	3664.7	429.4
20	0		8.384	$(13.41)_4$	464.9	15.52
40	0		0		0.00011	0
60	0		0		0	0
100	0		0		0	—

Table 6. Fractional errors $\times 10^5$ for $F = (1-x)^{-2}\exp(-(1-x)^{-1})$

n	T_1		T_3		T_5		T_∞
6	−403.8	$(-1.454)_2$	−706.5	$(-9.156)_4$	−2813.0	$(-1312.0)_6$	−2878.0
8	−242.2	$(-1.550)_2$	232.4	$(9.522)_4$	− 404.2	$(-1059.0)_6$	− 760.1
10	− 89.78	$(-0.897)_2$	− 71.83	$(-7.183)_4$	288.4	$(2884.0)_6$	− 178.5
12	− 47.36	$(-0.682)_2$	15.00	$(3.112)_4$	− 64.12	$(-1915.0)_6$	18.25
16	− 31.83	$(-0.815)_2$	0.2368	$(1.552)_4$	4.178	$(700.8)_6$	− 9.824
20	− 21.24	$(-0.850)_2$	− 0.3258	$(-5.257)_4$	0.9393	$(601.1)_6$	− 2.794
40	− 5.209	$(-0.833)_2$	− 0.01958	$(-4.968)_4$	0.00021	$(8.583)_6$	− 0.00142
60	− 2.314	$(-0.833)_2$	− 0.00387	$(-5.018)_4$	0		0
100	0		0		0		—

they are markedly in accordance with expectations. For example (Table 4) since $\sin(\pi x)$ already behaves as x and $1-x$ at the boundaries the transformations T_2 and T_4 carry it to the same state as T_3 and T_5 in the ordinary case.

In Table 5, $\exp(-100(x-0.5)^2)$ is a very peaked function, and it is clear that the transformations each make it more peaked. Clearly the integral will not be accurate until the peak is accurately integrated.

In Table 7, the function F already has all derivatives zero at both ends, and thus the transformations do not improve the errors.

Table 7. Fractional errors $\times 10^5$ for $F = \exp(-x^{-1} - (1-x)^{-1})$

n	T_1		T_3
6	-361.2	$(-1.300)_2$	-1688.7
8	6.344	$(406.0)_2$	107.8
10	20.17	$(0.2017)_2$	$-$ 5.698
12	4.436	$(0.0638)_2$	7.623
16	$-$ 0.7004	$(-0.00179)_2$	0.2687
20	$-$ 0.0379	$(-0.00015)_2$	0.04303
40	0		0
60	0		0
100	0		—

In Table 6, the integral is in fact $\int_0^\infty e^{-r}\,dr$, transformed by $r = x(1-x)^{-1}$ to bring its range to [0, 1]. Then though all derivatives are zero at $x=1$ substantial improvement is still obtained, as would be expected, since the transformations reduce the derivatives at $x=0$.

It is of interest to note that the transformation T_∞ gives results as accurate as the others from $n=16$ upwards, and at $n=40$, is giving the best results, all results being in the region of round-off error.

The small point that, since in the Eq. (4), in the practical applications

$$0.5(G(0)+G(1))=0 \tag{5}$$

there are only $(n-1)$ points of evaluation for n intervals, can become more important in many dimensions where only $(n-1)^M$ points are required.

The advantages and simplicity of this procedure as a first step, possible for one dimensional, but very markedly for many dimensions, does not appear to have been widely appreciated. It appears quite possible that combinations of this procedure with diophantine or similar systems of points [Haselgrove (1961), Conroy (1967)], might be one of the most effective methods for difficult many dimensional integrals. The work of Sag and Szekeres could probably be regarded as a special procedure of this type. In the diophantine approach, it is uncertain how much developments to improve accuracy have in the past been expended against boundary errors, more easily removed here, and how much against the interior integration. The freedom to adjust more effectively for just the second source of error might improve such methods considerably. It is considered there are two main sources of error: the boundary corrections, here removed; and the effects of integrating bulges in the interior by finite points. The result for the narrow gaussian curve (Table 5) gives a measure of the errors due to a bulge of width 0.2 and could be scaled to give a rough estimate for any suspected interior bulge effect.

It may be noted that such methods, especially T_∞, can be used to integrate functions which have integrable singularities, e.g.

$$x^{-0.5} + x^{-0.8} + (1-x)^{-0.95}.$$

Simple example of such cases are sometimes cited as being appropriate to Gauss point quadrature. But this might necessitate elaborate calculation of points for each integral. In other simpler cases Gauss point quadrature gives high accuracy but requires rather stringent knowledge that the integrand is very similar to a moderate finite expansion in terms of a particular type of function. This and other aspects practically exclude any general application of Gauss point procedures to more than one or two dimensions.

The above tables provide a means of estimating the errors for given points per dimension in many dimensional integrals after the boundary reduction transformations have been applied. In the simplest application the latter provide a very effective and simple way of reducing the integration to the evaluation of $(n-1)$ equally spaced points per dimension. It is to be hoped that further efficiency will be obtained by use of these transformations with other improved point systems.

References

1. Boys, S. F., Handy, N. C.: Proc. Roy. Soc. (London) A 311, 309 (1969)
2. Boys, S. F., Rajagopal, P.: Adv. Quantum Chem. **2**, 1 (1965)
3. Conroy, H.: J. Chem. Phys. **47**, 5307 (1967)
4. Haselgrove, C. B.: Math. Comp. **15**, 323 (1961)
5. Krylov, V. I.: Approximate calculation of integrals, p. 215. New York: MacMillan 1962
6. Sag, T. W., Szekeres, G.: Math. Comp. **18**, 245 (1964)
7. Whittaker, E. T., Robinson, G.: Calculus of observations, 2nd Ed., p. 134. London: Blackie 1937

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