A PORTABLE SUBPROGRAM FOR THE HIGH ORDER APPROXIMATION OF INTEGRALS USING EQUISPACED NODES

by

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INTRODUCTION:

The approximation of integrals using data from equispaced abscissae is an extremely common computational problem. Often such equispaced grids occur as being natural to computational models or to the taking of measurements. If an integral of a function specified only on this grid need be approximated, then several alternatives are available. The first is to use a standard quadrature method such as the composite trapezoidal or composite Simpson's rule. A second is to apply an appropriate Newton - Cotes formula. A third is to determine a function interpolating the given data, then integrate this interpolating function either exactly or by using an automatic quadrature method.

The first approach (i.e. trapezoidal or Simpson's rule) is sound but may not be sufficiently accurate for smooth functions. Furthermore, Simpson's rule is only defined when the number of abscissae is odd. The second approach requires knowledge of a Newton - Cotes formula. The set of quadrature weights for these formulae depend upon the number of abscissae and thus a separate rule must be available for every such number. The portability of programs including such weights is limited because of the varied allowable representations of constants on different computers and different compilers. Furthermore, the computational accuracy of such high order methods is often significantly effected by cancellation errors due to the presence of large weights of opposite signs. The third approach, that of first interpolating and then integrating the interpolant, occasionally is useful but can be quite inefficient.

The approach presented here results in a very short (about 20 executable FORTRAN lines) and portable subprogram with the capability of performing very accurate estimates of integrals.

METHOD:

The method employed appears to be originally due to Romberg [5], although it is more general than the algorithm traditionally associated with his name. This classical Romberg algorithm produces a sequence of composite trapezoidal rule approximations to the integral obtained by successive bisection of the interval of integration. This is usually used in an automatic quadrature method (i.e. one that can evaluate the integrand at any point in the interval of integration) but could be applied to the finite grid situation, if the number of abscissae is a power of two plus one. If the number of abscissae is not of such a form, the bisection process must be modified.

Let n denote the number of abscissae; thus n - 1 is the number of subintervals. If j is any integer that devides n - 1, then a composite trapezoidal rule could be applied by grouping together sets of j subintervals (i.e. by using ordinates with indices 1, j + 1, 2j + 1,...,n in the rule). Thus such a trapezoidal sum could be formed for every integer divisor of n - 1 (beginning with n - 1, and passing down to 1) and then Richardson extrapolation could be applied to the sequence. For example, with n = 13 abscissae (i.e. 12 subintervals), trapezoidal rules would be employed with sets of 12, 6, 4, 3, 2, and 1 subintervals. With n = 17, we have the traditional Romberg bisection process and the sequence of subintervals is 16, 8, 4, 2, and 1. Notice that with the smaller number 13, six trapezoidal sums can be formed compared to only 5 with n = 17. This allows one additional level of extrapolation.

In [2], Bulirsch presents the general extrapolation process for a sequence of trapezoidal sums. Using his results, we suggest the following algorithm:

1. Let $n_1, n_2, \ldots, n_m$ be the divisors of n - 1 in descending order (i.e. $n_1 = n - 1, \ldots n_m = 1$).
2. For k = 1, 2,..., m, obtain the trapezoidal sum T_1^k using

groups of n_k subintervals (i.e. using ordinates with indices $1, n_k + 1, \ldots, n$).

3. For $i = 1, \ldots, m - 1$ and for $k = 1, \ldots, m - i$, extrapolate by setting

$$T_{i+1}^{\ k} = \frac{T_i^{\ k+1} - (n_{k+1}/n_k)^2\, T_i^{\ k}}{1 - (n_{k+1}/n_k)^2}$$

4. The final value $T_m^{\ 1}$ is the approximation to the integral.

Although it appears that $m(m + 1)/2$ locations of storage are required for the T array, actually only m locations are necessary if quantities are properly over-written. (The present implementation uses an additional m locations for the storage of $n_1^{\ 2}, \ldots, n_m^{\ 2}$.)

According to Bulirsch [2], if f, the function specified on the equispaced abscissae, has 2m continuous derivatives on [a,b], the interval of integration, then the error satisfies

$$\int_a^b f(x)dx - T_m^{\ 1} = \frac{(-1)^m (b - a)^{2m+1} B_{2m}}{n_1^{\ 2} \ldots n_m^{\ 2}\ (2m)!}\ f^{(2m)}\ (\xi)$$

for some $\xi \varepsilon$ [a,b], where B_{2m} is the 2mth Bernoulli number (the first relevant ten of which are $B_2 = 1/6$. $B_4 = -1/30$, $B_6 = 1/42$, $B_8 = -1/30$, $B_{10} = 5/66$, $B_{12} = -691/2730$, $B_{14} = 7/6$, $B_{16} = -3617/510$, $B_{18} = 43{,}867/798$, $B_{20} = -174{,}611/330$).
This expression can be simplified, omitting all reference to the divisors $n_1, \ldots, n_m$, by the following observation:

If n_i divides $n - 1$ so does $(n - 1)/n_i$ and these two divisors are either distinct or $n_i = \sqrt{n - 1}$. If n_i and $(n - 1)/n_i$ are distinct then $n_i^{\ 2}((n - 1)/n_i)^2 = (n - 1)^2$. If $n_i = \sqrt{n - 1}$ then $n_i^{\ 2} = n - 1$. Thus we may conclude that the product $n_i^{\ 2} \ldots . n_m^{\ 2} = (n - 1)^m$.

Using this, we express the error expression in three alternative ways:

$$ {}_a\int^b f(x)dx - T_m^{\ 1} = \frac{(-1)^m (b-a)^{2m+1}\ B_{2m}}{(n-1)^m\ (2m)!}\ f^{(2m)}(\xi), $$

$$ = \frac{(-1)^m (b-a)^{m+1}\ h^m\ B_{2m}}{(2m)!}\ f^{(2m)}(\xi), $$

$$ = \frac{(-1)^m (n-1)^m\ h^{2m+1}\ B_{2m}}{(2m)!}\ f^{(2m)}(\xi), $$

where $h = (b - a)/(n - 1)$, the distance between adjacent abscissae (i.e. the "mesh width"). We may conclude that the method is of order $2m - 1$ (since it is exact for polynomials of that order) and that for fixed n, if $h \to o$ then the error is $O(h^{2m+1})$.

At least two questions arise about this method: does it have favorable computational properties and what is the effect of applying it to functions having less than 2m continuous derivatives? For the first, it can be shown that the method employed with finite precision arithmetic is equivalent to using exact arithmetic on slightly perturbed initial data. A related question is: although the final approximation is not computed this way, it is possible to compute it by taking some combination of given function values with certain weights(i.e. as traditional quadrature rules). If this were done, would any of these weights be negative? The answer is yes. In fact about 10% of the rules corresponding to values of n from 2 to 500 have negative weights (specifically n = 127, 281, 379 and whenever n - 1 is a multiple of 12 or 30). A more important question is whether the weights grow (causing severe cancellation errors). We offer no proof but the conjecture is that they are either bounded or growing extremely slowly. Computation of the weights of all rules through 500 shows them to have sums of absolute values less than 2.1 (where they have been normalized to have sum equal to 1). Newton - Cotes formulae, alternatively, have negative weights for n = 9 and all $n \geq 11$ (see Bernstein [1]), and these weights become unbounded. According to the estimates of Kusmin[4], the 50 point Newton - Cotes formula has one weight larger than 10^{22} and the 500 point formula has a weight larger than 10^{2988}. Thus the new method achieves high order accuracy without suffering the instabilities of the Newton - Cotes formulae. It is interesting to note that although no weights are stored, the new method is equivalent to Newton - Cotes for n = 2, 3, 4, 5, and 7.

The second question (i.e. what is the effect of this high order method on functions with less than 2m continuous derivatives) cannot be precisely answered. It is certainly the case that for a given function on a given grid a very low order method may be more accurate than a high order method. However, the situation in integration is not like that in interpolation, where a high order, polynomial based formula applied to an equispaced grid often produces disastrous results. Integration is a "smoothing" process, unlike interpolation, and often a high order quadrature formula, when applied to a function with only several continuous derivatives, yields a result about as accurate as the low order formula (see Davis and Rabinowitz [3], p. 26).

As a test of this claim, experiments were made with three test functions. The first is actually discontinuous ($f_1(x) = 1$, $x < \sqrt{2}/2$,; $f(x) = 0$, $x \geq \sqrt{2}/2$), the second has unbounded first derivative ($f_2(x) = \sqrt{x}$), and the third has unbounded second derivative ($f_3(x) = x^{3/2}$). All were integrated from 0 to 1, using from 2 to 50 points, and applying composite trapezoidal, composite Simpson's (for odd n), and the high order method. The results are given in tables 2, 3, and 4. We notice that, for the discontinuous function, the trapezoidal rule has smaller error than the high order method on about 53% of the trials and Simpson's rule has smaller error on about 58% of the trials. On the other two functions neither trapezoidal rule nor Simpson's rule ever had smaller error than the high order method.

Before describing the testing of the new subprogram, it is instructive to consider exactly what the order of this method is for various values of n. As previously mentioned, the order is one less than the number of divisors of n - 1.

This number may be computed easily by performing a prime factor decomposition of $n - 1$ as $p_1^{k_1} p_2^{k_2} \ldots p_m^{k_r}$ (where $p_1, \ldots, p_r$ are distinct primes). The number of divisors of $n - 1$ is $(k_1 + 1) \cdot (k_2 + 1) \ldots (k_r + 1)$. The order of the method for values of n from 2 to 500 is given in tables 1a and 1b. Notice that for $n > 2$ the order is always at least 3 (and is exactly three if and only if $n - 1$ is prime). The subprogram requires storage with length twice the number of divisors. This number may be computed using the above or simply bounded by 2n.

TESTING:

Besides the tests mentioned in the previous section, the FORTRAN function HIORDQ, implementing the high order integration method, was tested on five other functions suggested in Davis and Rabinowitz [3]. These include $f_4(x) = 1/(1 + x)$, $f_5(x) = 1/(1 + x^4)$, $f_6(x) = 1/(1 + e^x)$, $f_7(x) = x/(e^x - 1)$, and $f_8(x) = 2/(2+\sin(10\pi x))$. All were integrated from 0 to 1 using values of n from 2 to 50. The results are presented in tables 5 - 9, respectively, and the errors from trapezoidal and Simpson's methods are included for comparison. The tests were performed on the CDC 6400 at the University of Texas at Austin. This machine has nearly 15 digits of precision.

Notice that for integrands f_4 through f_7, the high order method always had smaller error than trapezoidal or Simpson's rules except for f_5 and $n = 5$ (and, of course, for all integrands with $n = 2$ and 3 where the method is the same as trapezoidal and Simpson's rule, respectively). Often the errors with the high order method are several powers of 10 smaller than those with the other two. The last integrand, f_8, shows the well knows effect of applying trapezoidal rule to periodic functions being integrated over their periods (or multiples thereof). In this case HIORDQ never returned more accurate results than trapezoidal or Simpson's rules and Simpson's rule was more accurate than trapezoidal on only two values of n (23 and 47). This provides additional support for the use of trapezoidal rule in periodic situations.

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		51	11	101	17	151	23	201	23
2	1	52	7	102	3	152	3	202	7
3	3	53	11	103	15	153	15	203	7
4	3	54	3	104	3	154	11	204	7
5	5	55	15	105	15	155	15	205	23
6	3	56	7	106	15	156	7	206	7
7	7	57	15	107	7	157	23	207	7
8	3	58	7	108	3	158	3	208	11
9	7	59	7	109	23	159	7	209	19
10	5	60	3	110	3	160	7	210	7
11	7	61	23	111	15	161	23	211	31
12	3	62	3	112	7	162	7	212	3
13	11	63	7	113	19	163	19	213	11
14	3	64	11	114	3	164	3	214	7
15	7	65	13	115	15	165	11	215	7
16	7	66	7	116	7	166	15	216	7
17	9	67	15	117	11	167	7	217	31
18	3	68	3	118	11	168	3	218	7
19	11	69	11	119	7	169	31	219	7
20	3	70	7	120	7	170	5	220	7
21	11	71	15	121	31	171	15	221	23
22	7	72	3	122	5	172	11	222	7
23	7	73	23	123	7	173	11	223	15
24	3	74	3	124	7	174	3	224	3
25	15	75	7	125	11	175	15	225	23
26	5	76	11	126	7	176	11	226	17
27	7	77	11	127	23	177	19	227	7
28	7	78	7	128	3	178	7	228	3
29	11	79	15	129	15	179	7	229	23
30	3	80	3	130	7	180	3	230	3
31	15	81	19	131	15	181	35	231	15
32	3	82	9	132	3	182	3	232	15
33	11	83	7	133	23	183	15	233	15
34	7	84	3	134	7	184	7	234	3
35	7	85	23	135	7	185	15	235	23
36	7	86	7	136	15	186	7	236	7
37	17	87	7	137	15	187	15	237	11
38	3	88	7	138	3	188	7	238	7
39	7	89	15	139	15	189	11	239	15
40	7	90	3	140	3	190	15	240	3
41	15	91	23	141	23	191	15	241	39
42	3	92	7	142	7	192	3	242	3
43	15	93	11	143	7	193	27	243	11
44	3	94	7	144	7	194	3	244	11
45	11	95	7	145	29	195	7	245	11
46	11	96	7	146	7	196	15	246	11
47	7	97	23	147	7	197	17	247	15
48	3	98	3	148	11	198	3	248	7
49	19	99	11	149	11	199	23	249	15
50	5	100	11	150	3	200	3	250	7

TABLE 1a: Order of Method for n=2,...,250

251	15	301	35	351	23	401	29	451	35
252	3	302	7	352	15	402	3	452	7
253	35	303	7	353	23	403	15	453	11
254	7	304	7	354	3	404	7	454	7
255	7	305	19	355	15	405	11	455	7
256	15	306	7	356	7	406	19	456	15
257	17	307	23	357	11	407	15	457	31
258	3	308	3	358	15	408	7	458	3
259	15	309	23	359	7	409	31	459	7
260	7	310	7	360	3	410	3	460	15
261	23	311	15	361	47	411	15	461	23
262	11	312	3	362	5	412	7	462	3
263	7	313	31	363	7	413	11	463	31
264	3	314	3	364	11	414	7	464	3
265	31	315	7	365	23	415	23	465	19
266	7	316	23	366	7	416	7	466	15
267	15	317	11	367	15	417	23	467	7
268	7	318	3	368	3	418	7	468	3
269	11	319	15	369	19	419	15	469	35
270	3	320	7	370	11	420	3	470	7
271	31	321	27	371	15	421	47	471	15
272	3	322	7	372	7	422	3	472	7
273	19	323	15	373	23	423	7	473	15
274	15	324	7	374	3	424	11	474	7
275	7	325	29	375	15	425	15	475	15
276	11	326	11	376	15	426	11	476	11
277	23	327	7	377	15	427	15	477	23
278	3	328	7	378	7	428	7	478	11
279	7	329	15	379	31	429	11	479	7
280	11	330	7	380	3	430	15	480	3
281	31	331	31	381	23	431	15	481	47
282	3	332	3	382	7	432	3	482	7
283	15	333	11	383	7	433	39	483	7
284	3	334	11	384	3	434	3	484	15
285	11	335	7	385	31	435	15	485	17
286	15	336	7	386	15	436	15	486	7
287	15	337	39	387	7	437	11	487	23
288	7	338	3	388	11	438	7	488	3
289	35	339	11	389	11	439	15	489	15
290	5	340	7	390	3	440	3	490	7
291	15	341	23	391	31	441	31	491	23
292	7	342	7	392	7	442	17	492	3
293	11	343	23	393	23	443	15	493	23
294	3	344	7	394	7	444	3	494	7
295	23	345	15	395	7	445	23	495	15
296	7	346	15	396	7	446	7	496	23
297	15	347	7	397	35	447	7	497	19
298	15	348	3	398	3	448	7	498	7
299	7	349	23	399	7	449	27	499	15
300	7	350	3	400	15	450	3	500	3

TABLE 1b: Order of Method for n=251,...,500

FUNCTION 1

N	HIORDQ	TRAPEZOIDAL	SIMPSONS
2	-2.07E-01	-2.07E-01	
3	1.26E-01	4.29E-02	1.26E-01
4	1.68E-01	1.26E-01	
5	-1.40E-01	-8.21E-02	-1.24E-01
6	1.23E-03	-7.11E-03	
7	-1.31E-02	4.29E-02	1.51E-02
8	-6.13E-02	-6.42E-02	
9	1.19E-02	-1.96E-02	1.23E-03
10	-8.57E-04	1.51E-02	
11	6.36E-02	4.29E-02	5.96E-02
12	-2.38E-02	-2.53E-02	
13	-7.16E-02	1.23E-03	-1.27E-02
14	2.50E-02	2.37E-02	
15	-1.51E-02	-2.85E-02	-1.66E-02
16	-3.59E-03	-7.11E-03	
17	2.37E-02	1.16E-02	2.21E-02
18	2.90E-02	2.82E-02	
19	-2.44E-02	-1.27E-02	-2.19E-02
20	4.00E-03	3.42E-03	
21	4.07E-03	1.79E-02	9.56E-03
22	-8.43E-03	-1.66E-02	
23	5.36E-03	-2.56E-03	5.01E-03
24	1.07E-02	1.03E-02	
25	-4.55E-02	-1.96E-02	-2.66E-02
26	-7.12E-03	-7.11E-03	
27	-2.17E-03	4.43E-03	-1.98E-03
28	1.53E-02	1.51E-02	
29	-3.68E-03	-1.07E-02	-4.73E-03
30	3.61E-05	-2.10E-04	
31	3.10E-02	9.56E-03	1.51E-02
32	-1.34E-02	-1.36E-02	
33	-1.20E-02	-3.98E-03	-9.19E-03
34	9.23E-03	5.01E-03	
35	8.50E-03	1.35E-02	8.58E-03
36	-2.14E-03	-7.11E-03	
37	1.40E-02	1.23E-03	5.86E-03
38	9.27E-03	9.11E-03	
39	-1.42E-02	-9.74E-03	-1.41E-02
40	-5.34E-03	-1.98E-03	
41	2.65E-03	5.39E-03	1.23E-03
42	-1.19E-02	-1.20E-02	
43	5.75E-04	-4.73E-03	-7.58E-04
44	2.31E-03	2.20E-03	
45	1.32E-02	8.80E-03	1.26E-02
46	-6.25E-03	-7.11E-03	
47	-4.24E-03	-5.85E-04	-4.21E-03
48	5.76E-03	5.66E-03	
49	8.74E-03	-9.19E-03	-5.72E-03
50	-1.72E-03	-3.03E-03	

TABLE 2: Error for Integration of

$f_1(x) = 1$ if $x\sqrt{2}/2$, $= 0$ if $x \geq \sqrt{2}/2$.

FUNCTION 2

N	HIORDQ	TRAPEZOIDAL	SIMPSONS
2	-1.67E-01	-1.67E-01	
3	-2.86E-02	-6.31E-02	-2.86E-02
4	-1.90E-02	-3.54E-02	
5	-8.91E-03	-2.34E-02	-1.01E-02
6	-1.07E-02	-1.69E-02	
7	-4.37E-03	-1.30E-02	-5.52E-03
8	-7.12E-03	-1.04E-02	
9	-3.06E-03	-8.54E-03	-3.59E-03
10	-3.47E-03	-7.19E-03	
11	-2.29E-03	-6.16E-03	-2.57E-03
12	-4.01E-03	-5.35E-03	
13	-1.42E-03	-4.71E-03	-1.95E-03
14	-3.22E-03	-4.19E-03	
15	-1.44E-03	-3.76E-03	-1.55E-03
16	-1.48E-03	-3.39E-03	
17	-1.07E-03	-3.09E-03	-1.27E-03
18	-2.25E-03	-2.82E-03	
19	-8.22E-04	-2.59E-03	-1.06E-03
20	-1.94E-03	-2.39E-03	
21	-7.32E-04	-2.22E-03	-9.08E-04
22	-9.42E-04	-2.07E-03	
23	-7.60E-04	-1.93E-03	-7.87E-04
24	-1.49E-03	-1.81E-03	
25	-4.92E-04	-1.70E-03	-6.90E-04
26	-9.42E-04	-1.60E-03	
27	-5.97E-04	-1.51E-03	-6.12E-04
28	-6.64E-04	-1.42E-03	
29	-4.58E-04	-1.35E-03	-5.48E-04
30	-1.08E-03	-1.28E-03	
31	-3.64E-04	-1.22E-03	-4.94E-04
32	-9.89E-04	-1.16E-03	
33	-3.79E-04	-1.11E-03	-4.48E-04
34	-4.99E-04	-1.06E-03	
35	-4.03E-04	-1.01E-03	-4.09E-04
36	-5.14E-04	-9.70E-04	
37	-2.68E-04	-9.30E-04	-3.76E-04
38	-7.72E-04	-8.93E-04	
39	-3.42E-04	-8.59E-04	-3.47E-04
40	-3.92E-04	-8.26E-04	
41	-2.53E-04	-7.96E-04	-3.21E-04
42	-6.68E-04	-7.67E-04	
43	-2.27E-04	-7.40E-04	-2.98E-04
44	-6.25E-04	-7.15E-04	
45	-2.39E-04	-6.91E-04	-2.78E-04
46	-2.75E-04	-6.68E-04	
47	-2.58E-04	-6.47E-04	-2.60E-04
48	-5.51E-04	-6.26E-04	
49	-1.73E-04	-6.07E-04	-2.44E-04
50	-3.82E-04	-5.89E-04	

TABLE 3: Error for Integration of $f_2(x) = \sqrt{x}$.

FUNCTION 3

N	HIORDQ	TRAPEZOIDAL	SIMPSONS
2	1.00E-01	1.00E-01	
3	2.37E-03	2.68E-02	2.37E-03
4	1.29E-03	1.23E-02	
5	3.03E-04	7.02E-03	4.32E-04
6	5.68E-04	4.54E-03	
7	8.73E-05	3.18E-03	1.58E-04
8	3.20E-04	2.35E-03	
9	4.96E-05	1.81E-03	7.72E-05
10	7.06E-05	1.44E-03	
11	3.13E-05	1.17E-03	4.43E-05
12	1.44E-04	9.70E-04	
13	1.29E-05	8.17E-04	2.81E-05
14	1.07E-04	6.98E-04	
15	1.51E-05	6.03E-04	1.91E-05
16	1.58E-05	5.26E-04	
17	8.62E-06	4.63E-04	1.37E-05
18	6.53E-05	4.11E-04	
19	5.31E-06	3.67E-04	1.02E-05
20	5.32E-05	3.30E-04	
21	4.42E-06	2.98E-04	7.86E-06
22	7.74E-06	2.71E-04	
23	5.39E-06	2.47E-04	6.19E-06
24	3.73E-05	2.26E-04	
25	2.18E-06	2.08E-04	4.98E-06
26	9.57E-06	1.92E-04	
27	3.64E-06	1.78E-04	4.08E-06
28	4.44E-06	1.65E-04	
29	2.07E-06	1.53E-04	3.39E-06
30	2.41E-05	1.43E-04	
31	1.33E-06	1.34E-04	2.85E-06
32	2.13E-05	1.25E-04	
33	1.52E-06	1.18E-04	2.43E-06
34	2.81E-06	1.11E-04	
35	1.92E-06	1.04E-04	2.09E-06
36	3.04E-06	9.85E-05	
37	7.92E-07	9.32E-05	1.81E-06
38	1.52E-05	8.82E-05	
39	1.47E-06	8.37E-05	1.58E-06
40	1.91E-06	7.95E-05	
41	7.41E-07	7.56E-05	1.39E-06
42	1.25E-05	7.20E-05	
43	6.15E-07	6.86E-05	1.23E-06
44	1.14E-05	6.55E-05	
45	7.13E-07	6.26E-05	1.10E-06
46	9.30E-07	5.99E-05	
47	9.28E-07	5.73E-05	9.80E-07
48	9.64E-06	5.49E-05	
49	3.81E-07	5.27E-05	8.81E-07
50	2.41E-06	5.05E-05	

TABLE 4: Error for Integration of $f_3(x) = x^{3/2}$.

FUNCTION 4

N	HIORDQ	TRAPEZOIDAL	SIMPSONS
2	5.69E-02	5.69E-02	
3	1.30E-03	1.52E-02	1.30E-03
4	6.03E-04	6.85E-03	
5	2.74E-05	3.88E-03	1.07E-04
6	2.23E-04	2.49E-03	
7	8.82E-07	1.73E-03	2.26E-05
8	1.14E-04	1.27E-03	
9	2.97E-07	9.75E-04	7.35E-06
10	2.71E-06	7.70E-04	
11	1.26E-07	6.24E-04	3.05E-06
12	4.65E-05	5.16E-04	
13	6.50E-10	4.34E-04	1.48E-06
14	3.33E-05	3.70E-04	
15	3.36E-08	3.19E-04	8.03E-07
16	2.84E-08	2.78E-04	
17	1.36E-09	2.44E-04	4.72E-07
18	1.95E-05	2.16E-04	
19	6.40E-11	1.93E-04	2.95E-07
20	1.56E-05	1.73E-04	
21	3.66E-11	1.56E-04	1.94E-07
22	7.60E-09	1.42E-04	
23	5.61E-09	1.29E-04	1.33E-07
24	1.07E-05	1.18E-04	
25	1.31E-13	1.08E-04	9.38E-08
26	1.34E-07	1.00E-04	
27	2.89E-09	9.24E-05	6.81E-08
28	2.81E-09	8.57E-05	
29	5.15E-12	7.97E-05	5.07E-08
30	6.71E-06	7.43E-05	
31	2.49E-14	6.94E-05	3.85E-08
32	5.87E-06	6.50E-05	
33	2.36E-12	6.10E-05	2.97E-08
34	1.27E-09	5.74E-05	
35	9.91E-10	5.41E-05	2.33E-08
36	1.07E-09	5.10E-05	
37	0	4.82E-05	1.86E-08
38	4.12E-06	4.56E-05	
39	6.36E-10	4.33E-05	1.50E-08
40	6.52E-10	4.11E-05	
41	7.11E-15	3.91E-05	1.22E-08
42	3.36E-06	3.72E-05	
43	3.55E-15	3.54E-05	1.00E-08
44	3.05E-06	3.38E-05	
45	3.52E-13	3.23E-05	8.33E-09
46	4.09E-13	3.09E-05	
47	2.96E-10	2.95E-05	6.97E-09
48	2.56E-06	2.83E-05	
49	-7.11E-15	2.71E-05	5.88E-09
50	1.81E-08	2.60E-05	

TABLE 5: Error for Integration of $f_4(x) = 1/(1+x)$.

FUNCTION 5

N	HIORDQ	TRAPEZOIDAL	SIMPSONS
2	-1.17E-01	-1.17E-01	
3	1.05E-02	-2.14E-02	1.05E-02
4	4.10E-03	-9.35E-03	
5	-5.48E-04	-5.24E-03	1.41E-04
6	1.39E-03	-3.35E-03	
7	2.07E-05	-2.32E-03	2.31E-05
8	6.97E-04	-1.70E-03	
9	7.91E-06	-1.30E-03	8.06E-06
10	-4.07E-05	-1.03E-03	
11	3.21E-06	-8.34E-04	3.32E-06
12	2.80E-04	-6.89E-04	
13	-4.18E-07	-5.79E-04	1.60E-06
14	2.00E-04	-4.93E-04	
15	8.25E-07	-4.25E-04	8.67E-07
16	7.91E-07	-3.71E-04	
17	-1.37E-08	-3.26E-04	5.08E-07
18	1.17E-04	-2.88E-04	
19	-1.96E-08	-2.57E-04	3.17E-07
20	9.34E-05	-2.31E-04	
21	-2.35E-09	-2.08E-04	2.08E-07
22	1.91E-07	-1.89E-04	
23	1.34E-07	-1.72E-04	1.42E-07
24	6.37E-05	-1.58E-04	
25	-8.87E-10	-1.45E-04	1.00E-07
26	-1.69E-06	-1.33E-04	
27	6.85E-08	-1.23E-04	7.29E-08
28	6.83E-08	-1.14E-04	
29	-2.66E-10	-1.06E-04	5.42E-08
30	4.00E-05	-9.91E-05	
31	-9.38E-11	-9.26E-05	4.12E-08
32	3.50E-05	-8.67E-05	
33	-1.15E-10	-8.14E-05	3.18E-08
34	3.02E-08	-7.65E-05	
35	2.34E-08	-7.21E-05	2.49E-08
36	1.86E-08	-6.80E-05	
37	8.49E-12	-6.43E-05	1.98E-08
38	2.46E-05	-6.09E-05	
39	1.50E-08	-5.77E-05	1.60E-08
40	1.54E-08	-5.48E-05	
41	-7.46E-14	-5.21E-05	1.30E-08
42	2.00E-05	-4.96E-05	
43	-4.60E-12	-4.72E-05	1.07E-08
44	1.82E-05	-4.51E-05	
45	-1.58E-11	-4.30E-05	8.89E-09
46	8.87E-11	-4.12E-05	
47	6.97E-09	-3.94E-05	7.44E-09
48	1.52E-05	-3.77E-05	
49	-1.14E-13	-3.62E-05	6.28E-09
50	-2.20E-07	-3.47E-05	

TABLE 6: Error for Integration of $f_5(x) = 1/(1+x^4)$.

FUNCTION 6

N	HIORDQ	TRAPEZOIDAL	SIMPSONS
2	4.59E-03	4.59E-03	
3	-3.48E-05	1.12E-03	-3.48E-05
4	-1.53E-05	4.96E-04	
5	1.91E-07	2.79E-04	-2.00E-06
6	-5.47E-06	1.78E-04	
7	-1.44E-09	1.24E-04	-3.89E-07
8	-2.78E-06	9.08E-05	
9	-4.49E-10	6.95E-05	-1.22E-07
10	1.63E-08	5.49E-05	
11	-1.83E-10	4.45E-05	-5.00E-08
12	-1.13E-06	3.68E-05	
13	-4.44E-14	3.09E-05	-2.41E-08
14	-8.06E-07	2.63E-05	
15	-4.73E-11	2.27E-05	-1.30E-08
16	-3.49E-11	1.98E-05	
17	3.80E-13	1.74E-05	-7.61E-09
18	-4.71E-07	1.54E-05	
19	-8.88E-15	1.37E-05	-4.75E-09
20	-3.77E-07	1.23E-05	
21	-5.33E-15	1.11E-05	-3.12E-09
22	-9.05E-12	1.01E-05	
23	-7.74E-12	9.19E-06	-2.13E-09
24	-2.58E-07	8.41E-06	
25	-3.55E-15	7.72E-06	-1.50E-09
26	7.51E-10	7.12E-06	
27	-3.96E-12	6.58E-06	-1.09E-09
28	-3.31E-12	6.10E-06	
29	-1.78E-15	5.67E-06	-8.11E-10
30	-1.62E-07	5.29E-06	
31	0	4.94E-06	-6.15E-10
32	-1.42E-07	4.63E-06	
33	-7.11E-15	4.34E-06	-4.75E-10
34	-1.48E-12	4.09E-06	
35	-1.36E-12	3.85E-06	-3.73E-10
36	-1.16E-12	3.63E-06	
37	-7.11E-15	3.43E-06	-2.97E-10
38	-9.95E-08	3.25E-06	
39	-8.72E-13	3.08E-06	-2.39E-10
40	-7.59E-13	2.93E-06	
41	-1.78E-15	2.78E-06	-1.95E-10
42	-8.10E-08	2.65E-06	
43	-3.55E-15	2.52E-06	-1.60E-10
44	-7.37E-08	2.41E-06	
45	-1.42E-14	2.30E-06	-1.33E-10
46	-5.33E-15	2.20E-06	
47	-4.12E-13	2.10E-06	-1.11E-10
48	-6.17E-08	2.01E-06	
49	-1.07E-14	1.93E-06	-9.39E-11
50	9.94E-11	1.85E-06	

TABLE 7: Error for Integration of $f_6(x) = 1/(1+e^x)$.

FUNCTION 7

N	HIORDQ	TRAPEZOIDAL	SIMPSONS
2	1.35E-02	1.35E-02	
3	-1.05E-05	3.36E-03	-1.05E-05
4	-4.65E-06	1.49E-03	
5	1.01E-08	8.40E-04	-6.46E-07
6	-1.67E-06	5.38E-04	
7	-1.54E-11	3.73E-04	-1.27E-07
8	-8.53E-07	2.74E-04	
9	-4.86E-12	2.10E-04	-4.02E-08
10	8.85E-10	1.66E-04	
11	-1.99E-12	1.34E-04	-1.65E-08
12	-3.45E-07	1.11E-04	
13	3.55E-15	9.33E-05	-7.94E-09
14	-2.47E-07	7.95E-05	
15	-5.12E-13	6.86E-05	-4.29E-09
16	-3.94E-13	5.97E-05	
17	3.55E-15	5.25E-05	-2.51E-09
18	-1.45E-07	4.65E-05	
19	1.07E-14	4.15E-05	-1.57E-09
20	-1.16E-07	3.72E-05	
21	7.11E-15	3.36E-05	-1.03E-09
22	-1.03E-13	3.05E-05	
23	-7.82E-14	2.78E-05	-7.03E-10
24	-7.90E-08	2.54E-05	
25	0	2.33E-05	-4.96E-10
26	4.12E-11	2.15E-05	
27	-4.26E-14	1.99E-05	-3.60E-10
28	-3.55E-14	1.84E-05	
29	-3.55E-15	1.71E-05	-2.68E-10
30	-4.97E-08	1.60E-05	
31	0	1.49E-05	-2.03E-10
32	-4.35E-08	1.40E-05	
33	-7.11E-15	1.31E-05	-1.57E-10
34	-1.78E-14	1.23E-05	
35	-1.78E-14	1.16E-05	-1.23E-10
36	-7.11E-15	1.10E-05	
37	-1.07E-14	1.04E-05	-9.80E-11
38	-3.05E-08	9.82E-06	
39	-7.11E-15	9.31E-06	-7.89E-11
40	-1.42E-14	8.84E-06	
41	-7.11E-15	8.40E-06	-6.43E-11
42	-2.49E-08	8.00E-06	
43	7.11E-15	7.62E-06	-5.29E-11
44	-2.26E-08	7.27E-06	
45	-1.42E-14	6.94E-06	-4.39E-11
46	7.11E-15	6.64E-06	
47	-3.55E-15	6.35E-06	-3.68E-11
48	-1.89E-08	6.09E-06	
49	-7.11E-15	5.83E-06	-3.10E-11
50	5.47E-12	5.60E-06	

TABLE 8: Error for Integration of $f(x) = x/(e^x-1)$.

FUNCTION 8

N	HIORDQ	TRAPEZOIDAL	SIMPSONS
2	-1.55E-01	-1.55E-01	
3	-1.55E-01	-1.55E-01	-1.55E-01
4	1.84E-02	-8.54E-04	
5	8.23E-02	1.20E-02	6.75E-02
6	-1.55E-01	-1.55E-01	
7	-2.12E-02	-8.54E-04	-8.54E-04
8	3.22E-03	-2.27E-08	
9	-1.01E-02	6.14E-05	-3.91E-03
10	-1.22E-04	-1.17E-10	
11	-1.55E-01	-1.55E-01	-1.55E-01
12	1.29E-03	-6.11E-13	
13	4.53E-03	3.16E-07	2.85E-04
14	9.21E-04	7.11E-15	
15	-3.76E-04	-2.27E-08	-2.27E-08
16	3.04E-02	-8.54E-04	
17	4.21E-04	1.63E-09	-2.05E-05
18	5.37E-04	-7.11E-15	
19	-1.43E-04	-1.17E-10	-1.17E-10
20	4.30E-04	0	
21	9.20E-02	1.20E-02	6.75E-02
22	-3.59E-06	0	
23	-5.79E-05	-6.11E-13	-6.04E-13
24	2.93E-04	-7.11E-15	
25	1.28E-04	5.68E-14	-1.05E-07
26	6.70E-03	-4.41E-06	
27	-2.93E-05	1.42E-14	1.42E-14
28	-1.17E-06	7.11E-15	
29	-1.59E-05	7.11E-15	7.57E-09
30	1.84E-04	7.11E-15	
31	-3.87E-02	-8.54E-04	-8.54E-04
32	1.61E-04	-7.11E-15	
33	-4.32E-06	0	-5.44E-10
34	-4.96E-07	-7.11E-15	
35	-9.90E-06	0	0
36	-3.50E-03	-2.27E-08	
37	-2.76E-06	0	3.90E-11
38	1.13E-04	7.11E-15	
39	-6.32E-06	0	0
40	-2.46E-07	7.11E-15	
41	-2.31E-02	6.14E-05	-3.91E-03
42	9.21E-05	-7.11E-15	
43	-1.52E-06	-7.11E-15	1.42E-14
44	8.37E-05	-7.11E-15	
45	-7.79E-07	0	1.92E-13
46	3.72E-04	-1.17E-10	
47	-2.93E-06	-1.42E-14	-7.11E-15
48	7.01E-05	7.11E-15	
49	3.92E-07	-7.11E-15	-1.42E-14
50	-1.34E-06	0	

TABLE 9: Error for Integration of $f_8(x) = 2/(2 + \sin 10\pi x)$.

```
      FUNCTION HIORDQ (N, Y, DELT, WORK)
C
C                                 ALAN KAYLOR CLINE
C                                 DEPARTMENT OF COMPUTER SCIENCES
C                                 UNIVERSITY OF TEXAS AT AUSTIN
C
      INTEGER N
      REAL    Y(N), DELT, WORK(1)
C
C THIS FUNCTION APPROXIMATES THE INTEGRAL OF A FUNCTION
C SPECIFIED AS AN ARRAY OF ORDINATES CORRESPONDING TO
C EQUALLY SPACED ABSCISSAE ON THE INTERVAL OF INTEGRATION.
C THE METHOD APPLIES THE TRAPEZOIDAL RULE TO VARIOUS SUBSETS
C OF THE DATA (EACH CORRESPONDING TO AN INTEGER DIVISOR OF
C THE NUMBER OF ORDINATES MINUS ONE), THEN USES RICHARDSON
C EXTRAPOLATION TO YIELD A (HOPEFULLY) IMPROVED ESTIMATE OF
C THE INTEGRAL.
C
C ON INPUT--
C
C   N  CONTAINS THE NUMBER OF ORDINATES IN THE ARRAY,
C      (N .GE. 2).
C
C   Y  IS AN ARRAY OF LENGTH N CONTAINING THE ORDINATES. IT
C      IS ASSUMED THAT Y(I) CONTAINS THE FUNCTION VALUE AT
C      THE I-TH EQUALLY SPACED ABSCISSA,
C
C   DELT  CONTAINS THE SPACING BETWEEN ADJACENT ABSCISSAE.
C         THE INTEGRAL IS TAKEN FROM FIRST TO LAST ABSCISSA,
C         THUS THE INTERVAL OF INTEGRATION HAS LENGTH DELT *
C         (N-1). IF THE UPPER LIMIT OF INTEGRATION IS LESS
C         THAN THE LOWER LIMIT OF INTEGRATION, THEN DELT
C         SHOULD BE NEGATIVE.
C
C AND
C
C   WORK  IS AN ARRAY TO BE USED INTERNALLY FOR WORKSPACE.
C         ITS LENGTH SHOULD BE AT LEAST TWICE THE NUMBER OF
C         INTEGER DIVISORS OF N-1. (IF N-1 HAS A PRIME
C         FACTOR DECOMPOSITION
C
C           (P(1)**K(1)) * (P(2)**K(2)) * ... * (P(M)**K(M))
C
C         THEN 2*(K(1)+1)*(K(2)+1)* ... *(K(M)+1) LOCATIONS
C         ARE REQUIRED.) A LENGTH OF 2*N WILL ALWAYS
C         SUFFICE.
C
C ON OUTPUT--
C
C   HIORDQ RETURNS THE APPROXIMATE INTEGRAL
C
C AND N, Y, AND DELT ARE UNALTERED.
C
```

```
      NN = N
      NM1 = NN - 1
C
C DETERMINE INITIAL TRAPEZOIDAL RULE
C
      SUM1 = (Y(1) + Y(NN))/2.
      J = -1
      DO 3 K = 1,NM1
        NM1DK = NM1/K
C
C CHECK IF K DIVIDES N-1
C
        IF (NM1DK*K .NE. NM1) GO TO 3
C
C DETERMINE K-POINT TRAPEZOIDAL RULE
C
        SUM = -SUM1
        DO 1 I = 1,NN,NM1DK
    1     SUM = SUM + Y(I)
        J = J + 2
        WORK(J) = DELT*SUM*FLOAT(NM1DK)
        JP1 = J + 1
        WORK(JP1) = FLOAT(NM1DK*NM1DK)
        IF (K .EQ. 1) GO TO 3
C
C APPLY RICHARDSON EXTRAPOLATION
C
        DO 2 JJ = 3,J,2
          JBAK = JP1 - JJ
          FAC = WORK(JP1)/(WORK(JP1)-WORK(JBAK+1))
    2     WORK(JBAK) = WORK(JBAK+2)
     1                + FAC*(WORK(JBAK)-WORK(JBAK+2))
    3   CONTINUE
      HIORDQ = WORK(1)
      RETURN
      END
```