Numerical quadrature (supplement) : a comparison of available procedures at the Computing Centre of the Eindhoven University of Technology

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Numerical Quadrature (supplement)

A comparison of available procedures at the Computing Centre of the Eindhoven University of Technology

by

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Summary

Since the publication of the report on a comparison of Algol procedures for numerical quadrature, TH-Report 81-WSK-04, the contents of the NAG-Library with respect to automatic numerical quadrature have been altered. Two new procedures have been inserted: D01AHA and D01AJA.
The performance of these procedures has been evaluated and compared with some other procedures by the method described in the above mentioned report. The results are given in the present note which is to be considered a supplement of this report, and which therefore has the same title.

AMS Subject Classification: 65D30, 68B99

1. Introduction

In August 1981 we published a comparison test of Algol procedures for automatic numerical quadrature[1]. The set of tested procedures contained four procedures from the NAG-Library, Mark 7, namely D01AAA, D01ABA, D01ACA and D01AGA.

With the Mark 8 release D01AAA and D01ABA have been withdrawn, which is not surprising in view of the results in [1]. Furthermore, D01AGA will be withdrawn at Mark 9 and from the Fortran documentation it is clear that the same will occur to D01ACA in due course.

On the other hand, two new procedures have been inserted into the NAG-Library, namely D01AHA and D01AJA. We have tested the performance of these procedures by the method of [1]. In this note we report the results of the test.

For the framework of the test, the notations and the presentation of the results the reader is referred to [1], of which this note is to be seen as a supplement.

2. Description of the procedures

D01AHA is an adaptive modification of D01ACA. This implies, among others, that the endpoints of the interval of integration are not used. A relative accuracy must be supplied, but the documentation does not make clear which quantity this accuracy is related to. A limit to the number of function evaluations must also be given; in our test we have chosen the default limit of 10.000.

The accuracy indication is realized by the parameter IFAIL. The procedure also returns a rough estimate of the relative error achieved.

DO1AJA is an adaptive procedure, designed by Piessens and De Doncker, using Gauss 10-point and Kronrod 21-point rules. An absolute and a relative (to the integral) tolerance must be supplied; the procedure endeavours to satisfy either one. An upperbound to the number of subintervals must be given; in the test we have chosen the value 200.

The accuracy indication is realized by the parameter IFAIL. The procedure also returns an estimate of the modulus of the absolute error.
The documentation describes DO1AJA as the favourite routine for automatic integration in the cases where the integrand is known to be badly-behaved, or where its nature is completely unknown.
Other procedures may be more efficient, however, and may therefore be recommended in other cases.

3. Reliability and efficiency, numerical results

In this section we give the numerical results of the test on both procedures. For comparison the results of the procedures SIMPSONINT and DO1AGA are added.
The efficiency is recorded by the components of the Perron-Frobenius eigenvector of the reciprocal matrix E (cf.[1], p.19) normalized such that the component corresponding to DO1AHA equals 1, i.e., the components give the efficiency relative to DO1AHA.
For the complete efficiency tables, see the appendix, pp. 10-14.

Group 1. Smooth or well-behaved functions

Reliability table

	10^{-3}				10^{-6}				10^{-9}			
METHOD	0	1	2	3	0	1	2	3	0	1	2	3
3: SIMPSONINT	100				100				100			
8: DO1AHA	100				100				100			
9: DO1AJA	100				100				100			
11: DO1AGA	100				100				100			

Efficiency table

	SIMPSONINT	DO1AGA	DO1AHA	DO1AJA
10^{-3}	1.3	0.9	1	1.6
10^{-6}	3.1	1.1	1	1.5
10^{-9}	10.6	1.2	1	1.5

DO1AHA is more efficient than DO1AJA, and is at least as good as the other ones. So DO1AHA may be recommended.

Group 2. Functions with one or more sharp peaks within the interval.

Reliability table

	10^{-3}				10^{-6}				10^{-9}			
METHOD	0	1	2	3	0	1	2	3	0	1	2	3
3: SIMPSONINT	99			1	100				96			4
8: DO1AHA	87			13	99			1	73		1	26
9: DO1AJA	100				100				82	3	10	5
11: DO1AGA	73		11	16	99			1	84			16

Efficiency table

	SIMPSONINT	DO1AGA	DO1AHA	DO1AJA
10^{-3}	0.5	0.6	1	1.7
10^{-6}	1.5	0.6	1	1.5
10^{-9}	5.6	0.8	1	1.5

The reliability of DO1AJA is satisfactory. The 10% incorrectly computed integrals, and indicated as such, have IFAIL = 2, i.e., roundoff error prevents the requested tolerance from being achieved.
But notice the high reliability score of SIMPSONINT! This together with its efficiency score, except for $\varepsilon = 10^{-9}$, makes SIMPSONINT competitive.

Group 3. Functions with a singularity in (one of) the endpoints.

Reliability table

	10^{-3}				10^{-6}				10^{-9}			
METHOD	0	1	2	3	0	1	2	3	0	1	2	3
3: SIMPSONINT	100				100				95			5
8: DO1AHA	100				98			2	92			8
9: DO1AJA	100				100				100			
11: DO1AGA	99			1	97			3	98			2

Efficiency table

	SIMPSONINT	DO1AGA	DO1AHA	DO1AJA
10^{-3}	1.9	1.4	1	5.2
10^{-6}	2.9	2.4	1	4.9
10^{-9}	4.8	2.2	1	2.5

For this group DO1AHA is to be preferred on account of the efficiency score. Remember that the procedure does not make use of the endpoints of the interval of integration.

Group 4. Functions with a singularity within the open interval.

Reliability table

METHOD	10^{-3} 0	1	2	3	10^{-6} 0	1	2	3	10^{-9} 0	1	2	3
3: SIMPSONINT	100				100				95			5
8: DO1AHA	78			22	82			18	84			16
9: DO1AJA	100				98			2	97	1		2
11: DO1AGA	73		1	26	67	2	3	28	68	1	4	27

Efficiency table

	SIMPSONINT	DO1AGA	DO1AHA	DO1AJA
10^{-3}	0.4	0.5	1	2.3
10^{-6}	0.3	0.3	1	1.0
10^{-9}	0.6	0.4	1	1.0

The claim in the documentation that DO1AJA is especially suited to this group is not quite affirmed by the test, since SIMPSONINT is competitive with respect to reliability and significantly better than both DO1AHA and DO1AJA with respect to efficiency.

So we should recommend SIMPSONINT for problems of this type.

Group 5. Rapidly oscillating functions.

Reliability table

METHOD	10^{-3} 0	1	2	3	10^{-6} 0	1	2	3	10^{-9} 0	1	2	3
3: SIMPSONINT	85			15	93			7	79			21
8: D01AHA	95			5	100				93			7
9: D01AJA	100				100				90	6	4	
11: D01AGA	80		15	5	90		10		92		3	5

Efficiency table

	SIMPSONINT	D01AGA	D01AHA	D01AJA
10^{-3}	0.9	1.3	1	1.7
10^{-6}	2.9	1.4	1	1.5
10^{-9}	12.9	1.5	1	1.7

Both D01AHA and D01AJA are satisfactorily reliable and D01AJA somewhat more, indeed. By virtue of the efficiency scores D01AHA may be preferred.

Group 6. Pestfunctions.

The performance on the group of so-called pestfunctions may be summarized as follows.

With $\varepsilon = 10^{-3}$ the scores of successfully computed integrals are: SIMPSONINT 75%, D01AHA 73%, D01AJA 97%, while the efficiency of SIMPSON-INT is about four times as good as those of the other two which are more or less the same.

With $\varepsilon = 10^{-6}$ the scores are: SIMPSONINT 43%, D01AHA 50%, D01AJA 65% (of which 5% with IFAIL = 1 or 2). The real pestfunctions turn out to be 601 up to 604, 609 and 613. For the joint successfully computed integrals SIMPSONINT is the more efficient; about twice.

4. Relevancy of the accuracy indicators

As in [1] we also considered the relevance of the parameter IFAIL. With respect to D01AHA we can be very short. The value of IFAIL was in all cases but one zero, so it has in our opinion no significance at all.

D01AJA is so reliable that IFAIL hardly has to differ from zero. But when it did so, it gave in most cases the correct indication, especially in the unsuccessful cases of group 6.

After the documentation the parameter RELERR of D01AHA contains, on exit, a rough estimate of the relative error achieved. However, the significance of this parameter is doubtful since in the cases of interest, namely when the accuracy has not been achieved, the value of RELERR is mostly much smaller than the actual error, and therefore misleading.

The parameter ABSERR of D01AJA contains, on exit, an estimate of the modulus of the absolute error, which should be an upper bound for $|I - RESULT|$. This claim is affirmed by the results of our test.

5. Conclusion

The statement in the documentation of the NAG-Library that "D01AHA is likely to be more efficient, whereas D01AJA is somewhat more reliable ..." cf[2, Introduction-D01,p.7], is affirmed by the results of our test. With respect to reliability this assertion is based not only on the percentages of correctly computed integrals, but also on the relevance of the parameters IFAIL and ABSERR of D01AJA. In contrast, the corresponding para-

meters of DO1AHA did show no relevance at all in the test.
For smooth functions or functions with a singularity at an endpoint of the interval of integration DO1AHA is to be preferred because of its higher efficiency, whereas for functions the nature of which is unknown or which have a difficulty in an interior point DO1AJA is more reliable and therefore is recommended. But especially in the latter case (i.e. the groups 2 and 4) the performance of SIMPSONINT, a much simpler algorithm, is remarkably good!

References

[1] Geurts, A.J. and P.J. den Haan, Numerical Quadrature, A comparison of available procedures at the Computing Centre of the Eindhoven University of Technology, TH-Report 81-WSK-04.

[2] NAG ALGOL 60 Library Manual - Mark 8. Numerical Algorithm Group Ltd., Oxford, 1981.

Appendix. Efficiency tables

INPUT IDENTIFICATION : GROUP 1
EPS=@-3
NUMBER OF SELECTED INTEGRALS: 220

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		1.3	0.8	1.5	1.3	1.3	0.43
8: D01AHA	100		0.6	1.1	1.0	1.0	0.00
9: D01AJA	100	100		1.8	1.6	1.6	0.72
11: D01AGA	100	100	100		0.9	0.9	-0.15

CONSISTENCY:-4.851E-12

INPUT IDENTIFICATION : GROUP 1
EPS=@-6
NUMBER OF SELECTED INTEGRALS: 220

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		3.1	2.0	2.9	3.1	3.1	1.61
8: D01AHA	100		0.7	0.9	1.0	1.0	0.00
9: D01AJA	100	100		1.4	1.5	1.5	0.62
11: D01AGA	100	100	100		1.1	1.1	0.10

CONSISTENCY: 1.128E-07

INPUT IDENTIFICATION : GROUP 1
EPS=@-9
NUMBER OF SELECTED INTEGRALS: 220

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		10.6	7.0	8.6	10.6	10.6	3.41
8: D01AHA	100		0.7	0.8	1.0	1.0	0.00
9: D01AJA	100	100		1.2	1.5	1.5	0.60
11: D01AGA	100	100	100		1.2	1.2	0.32

CONSISTENCY: 0.

INPUT IDENTIFICATION : GROUP 2
EPS=@-3

NUMBER OF SELECTED INTEGRALS: 140

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		0.5	0.3	0.9	0.5	0.5	-0.94
8: D01AHA	87		0.6	1.6	1.0	1.0	0.00
9: D01AJA	99	87		3.0	1.7	1.7	0.80
11: D01AGA	73	66	74		0.6	0.6	-0.74

CONSISTENCY: 1.233E-04

INPUT IDENTIFICATION : GROUP 2
EPS=@-6

NUMBER OF SELECTED INTEGRALS: 140

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		1.5	1.0	2.3	1.5	1.5	0.56
8: D01AHA	99		0.7	1.6	1.0	1.0	0.00
9: D01AJA	100	99		2.4	1.5	1.5	0.58
11: D01AGA	99	99	99		0.6	0.6	-0.67

CONSISTENCY: 4.144E-07

INPUT IDENTIFICATION : GROUP 2
EPS=@-9

NUMBER OF SELECTED INTEGRALS: 136

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		5.6	3.7	7.2	5.7	5.6	2.50
8: D01AHA	76		0.7	1.2	1.0	1.0	0.00
9: D01AJA	87	74		1.9	1.5	1.5	0.61
11: D01AGA	87	74	82		0.8	0.8	-0.34

CONSISTENCY: 5.650E-05

INPUT IDENTIFICATION : GROUP 3
EPS=@-3
NUMBER OF SELECTED INTEGRALS: 200

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		1.9	0.4	1.4	1.9	1.9	0.96
8: D01AHA	100		0.2	0.7	1.0	1.0	0.00
9: D01AJA	100	100		3.8	5.2	5.2	2.39
11: D01AGA	99	99	99		1.4	1.4	0.45

CONSISTENCY: 6.071E-07

INPUT IDENTIFICATION : GROUP 3
EPS=@-6
NUMBER OF SELECTED INTEGRALS: 200

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		2.9	0.6	1.2	2.9	2.9	1.52
8: D01AHA	98		0.2	0.4	1.0	1.0	0.00
9: D01AJA	100	98		2.0	4.9	4.9	2.30
11: D01AGA	97	95	97		2.4	2.4	1.29

CONSISTENCY: 9.879E-07

INPUT IDENTIFICATION : GROUP 3
EPS=@-9
NUMBER OF SELECTED INTEGRALS: 200

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		4.7	1.9	2.2	4.8	4.8	2.27
8: D01AHA	87		0.4	0.4	1.0	1.0	0.00
9: D01AJA	95	92		1.1	2.5	2.5	1.33
11: D01AGA	93	90	98		2.3	2.2	1.17

CONSISTENCY: 8.417E-05

INPUT IDENTIFICATION : GROUP 4
EPS=@-3
NUMBER OF SELECTED INTEGRALS: 200

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		0.3	0.2	0.7	0.4	0.4	-1.50
8: D01AHA	78		0.5	1.9	1.0	1.0	0.00
9: D01AJA	99	78		4.4	2.3	2.3	1.18
11: D01AGA	73	55	72		0.5	0.5	-0.95

CONSISTENCY: 3.525E-04

INPUT IDENTIFICATION : GROUP 4
EPS=@-6
NUMBER OF SELECTED INTEGRALS: 200

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		0.3	0.3	0.8	0.3	0.3	-1.92
8: D01AHA	82		1.0	3.0	1.0	1.0	0.00
9: D01AJA	98	81		2.9	1.0	1.0	-0.01
11: D01AGA	68	58	67		0.3	0.3	-1.56

CONSISTENCY: 1.173E-04

INPUT IDENTIFICATION : GROUP 4
EPS=@-9
NUMBER OF SELECTED INTEGRALS: 199

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		0.6	0.6	1.6	0.6	0.6	-0.77
8: D01AHA	80		1.1	2.7	1.0	1.0	0.00
9: D01AJA	93	82		2.6	1.0	1.0	-0.07
11: D01AGA	68	56	67		0.4	0.4	-1.43

CONSISTENCY: 5.809E-05

INPUT IDENTIFICATION : GROUP 5
EPS=@-3
NUMBER OF SELECTED INTEGRALS: 200

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		0.9	0.5	0.7	0.9	0.9	-0.16
8: D01AHA	80		0.6	0.8	1.0	1.0	0.00
9: D01AJA	85	95		1.3	1.7	1.7	0.77
11: D01AGA	67	76	80		1.3	1.3	0.39

CONSISTENCY: 3.948E-04

INPUT IDENTIFICATION : GROUP 5
EPS=@-6
NUMBER OF SELECTED INTEGRALS: 200

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		2.8	1.9	2.2	2.9	2.9	1.52
8: D01AHA	93		0.7	0.7	1.0	1.0	0.00
9: D01AJA	93	100		1.0	1.5	1.5	0.58
11: D01AGA	82	90	90		1.4	1.4	0.48

CONSISTENCY: 7.583E-04

INPUT IDENTIFICATION : GROUP 5
EPS=@-9
NUMBER OF SELECTED INTEGRALS: 193

METHOD	3	8	9	11	REL.EFF.NUMBERS MEAN ROW SUM	EIG. VEC.	LOG. SCA.
3: SIMPSONINT		13.0	7.9	8.1	12.9	12.9	3.69
8: D01AHA	81		0.6	0.7	1.0	1.0	0.00
9: D01AJA	82	96		1.1	1.6	1.7	0.72
11: D01AGA	81	93	95		1.5	1.5	0.63

CONSISTENCY: 7.276E-05