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by Charles M. Goldstein
Lewis Research Center
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TECHNICAL PREPRINT prepared for Twenty-Fourth
Semiannual SHARE Meeting
Los Angeles, California, March 1, 1965

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## INTRODUCTION

The primary purpose of this paper is to describe a family of very powerful numerical integration techniques for use at the Lewis Research Center. The discussion and evaluation of these techniques will be of interest, however, at all computing centers where the techniques are not already receiving wide usage. Although the techniques are not new, or original, an appreciation of the savings in computor time that may be achieved by their application seems sadly lacking. In fact, a recent book[1] on "numerical methods and computor programming" discusses Simpson's Rule but not Gauss' formula.

A comparison is made between these techniques and a modified Simpson's Rule program, SIMPS1, written by Drs. T. Fessler and W. Ford of the Lewis Research Center. A brief description of SIMPS1 and how it is related to ordinary Simpson's Rule will be presented herein.

A description of the Fortran IV programs and their call vectors is given in the Appendix. The format presented herein is that of the Lewis Monitor Manual. These programs, with the exception of QUAD4, have been programmed by H. E. Renkel of the Lewis Research Center.

## GAUSSIAN QUADRATURE

### Gauss' Formula

According to Scarborough[2], "The most accurate of the quadrature formulas in ordinary use is known as Gauss' formula." This formula can be written in the following form:

$$\int_{-1}^{+1} f(x)dx = \sum_{\alpha=1}^{N} H_\alpha f(x_\alpha) \tag{1}$$

The normalization to the region (-1,+1) imposes no real restriction (in fact, the normalization is effected internally in the FORTRAN programs). The abscissas $x_\alpha$ and the weight coefficients $H_\alpha$ have prescribed values for each N. Kopal[3] discusses the evaluation of $x_\alpha$ and $H_\alpha$ for any given N.

The reason Gauss's formula has not received more complete acceptance is given by Ralston[4] (1960): "Until recently Gaussian type quadrature formulas were seldom used because in most cases the abscissas are irrational numbers, which, of course, makes them inconvenient for hand computation. However, on digital computers this argument has little weight . . ."

Gauss' formula (eq. (1)) has been programmed in single and double precision. These function subroutines and their call vectors are described in the appendix.

## Weight Functions

A series of formulas belonging to the Gaussian quadrature family is of the form

$$\int_a^b W(x)f(x)\ dx = \sum_{\alpha=1}^{N} H_\alpha f(x_\alpha) \tag{2}$$

where $W(x)$ is a given weight function. A list of the more common formulas of this type and their definition is given in table I. In the last column of table I the FORTRAN IV subprogram names are given. SQUAD1 and DSQUAD1 are subroutines. All the others are function subprograms. The prefix D denotes double precision programs. These subprograms are more fully described in the appendix.

To appreciate the desirability of QUAD2, it must be recognized that all commonly used integration formulas implicitly assume that the integrand may be approximated (over the region of integration) by a polynominal. Germane to the weight $\sqrt{x}$ it must also be recognized that no polynominal expansion in the independent variable can represent a curve that possesses an infinite derivative within the region of interest.

The comments for the case when the integrand has an infinite derivative apply even more so when the integrand is singular in the region of integration (viz., QUAD 3, QUAD 4).

Note that the formulas given herein are all open-ended formulas; that is, the integration formulas do not evaluate the integrand at the endpoints. This property will be used later to advantage when the integrand has an implicit singularity. For further properties of Gaussian quadrature consult reference 3.

The coefficients and abscissas of other weighted-Gaussian quadrature formulas are to be found in reference 5 and recent literature (such as the Journal of Mathematics of Computation).

## Multiple Integrations

It is often necessary to numerically integrate equations of the following type:

TABLE I. - GAUSSIAN QUADRATURE FORMULAS

| Quadrature formula names | | Reference | FORTRAN IV routine names[a] |
|---|---|---|---|
| Gauss | $\int_{-1}^{+1} f(x)\ dx = \sum_{\alpha=1}^{N} H_\alpha f(x_\alpha)$ | 3 | QUAD1, DQUAD1<br>SQUAD1, DSQUAD1 |
| $\sqrt{x}$ - Weighted Gaussian | $\int_{0}^{1} \sqrt{x}\ f(x) = \sum_{\alpha=1}^{N} H_\alpha f(x_\alpha)$ | 5 | QUAD2 |
| $\frac{1}{\sqrt{x}}$ - Weighted Gaussian | $\int_{0}^{1} \frac{f(x)}{\sqrt{x}}\ dx = \sum_{\alpha=1}^{N} H_\alpha f(x_\alpha)$ | 6 | QUAD3,DQUAD3 |
| Logarithmic Gaussian | $\int_{0}^{1} f(x) \ln x\ dx = \sum_{\alpha=1}^{N} H_\alpha f(x_\alpha)$ | (b) | QUAD4 |
| Gauss-Laguerre | $\int_{0}^{\infty} e^{-x} f(x)\ dx = \sum_{\alpha=1}^{N} H_\alpha f(x_\alpha)$ | 7 | QUAD5, DQUAD5 |
| Gauss-Hermite | $\int_{-\infty}^{+\infty} e^{-x^2} f(x)\ dx = \sum_{\alpha=1}^{N} H_\alpha f(x_\alpha)$ | 7 | QUAD6, DQUAD6 |

[a]See appendix.

[b]Private communication from Peter Sockol.

$$\int_{-1}^{+1} f(x) \int_{a(x)}^{b(x)} g(x,y)\, dy\, dx \tag{3}$$

Subroutines SQUAD1 and DSQUAD1 are presented in the appendix for this purpose.

## EVALUATION

Usually, a reasonable indication of the efficiency of a method for numerical integration is given by the number of times the integrand must be evaluated to achieve a particular accuracy. Table II presents the results of numerically integrating the integral

$$\int_{0}^{1} W(x)f(x)\, dx \tag{4}$$

for various weights $W(x)$ and functions $f(x)$ by SIMPS1 and the appropriate Gaussian quadrature formula. The singular integrands (examples 3, 4, 7 to 10, and 12 in table II) cannot, of course, be evaluated by Simpson's Rule to the singularity (here, zero) but can only be evaluated to within some $\epsilon$ of it. Results for $\epsilon = 10^{-4}$ and $\epsilon = 10^{-5}$ are presented in the table. $N_S$ denotes the number of times SIMPS1 evaluated the integrand. The error, in examples 1 to 12, is given in units of the eighth digit, and represents the absolute error. The Gaussian quadrature errors are tabulated for 3, 5, 7, 9, and 11 integration points, respectively. The last column in the table shows the ratio of $N_S$ to $N_G$ where $N_G$ represents the number of times the Gaussian quadrature needed to evaluate the integrand to achieve an error comparable to SIMPS1.

Examples 1 to 12 were chosen so that the integral could be performed exactly and an accurate absolute error could be obtained. Example 13 is an evaluation of the following integral:

$$\int_{0}^{1} \frac{e^{-10x}}{\sqrt{1 + \varphi(x)}} \ln \frac{\sqrt{1 + A} + \sqrt{1 + \varphi(x)}}{\sqrt{A} + \sqrt{\varphi(x)}}\, dx \tag{5}$$

where

$$\varphi(x) = x^2 + 3x^3$$

$$A = 0.013$$

This integral was encountered by the author in a recent problem and is included to show that even with a not too badly behaved integrand, the ratio $N_S/N_G$ may exceed 10.

TABLE II. - RESULTS OF EVALUATING $\int_0^1 W(x)\, f(x)\, dx$

| Example | W(x) | f(x) | SIMPS1 | | Gaussian quadratures | | | | | | $\frac{N_S}{N_G}$ |
|---|---|---|---|---|---|---|---|---|---|---|---|
| | | | $N_S$ | Error | Routine | Error | | | | | |
| | | | | | | 3 | 5 | 7 | 9 | 11 | |
| 1 | 1 | $1 + x$ | 5 | 0 | QUAD1 | 0 | 0 | 0 | 0 | -1 | 1.6 |
| 2 | $\sqrt{x}$ | | 49 | -10 | QUAD2 | 0 | 0 | 0 | 0 | 0 | 16 |
| 3 | $1/\sqrt{x}$ | | [a]117 | -4 | QUAD3 | -1 | 0 | -1 | -1 | -1 | 39 |
| 4 | $\ln x$ | | [a]97 | 1 | QUAD4 | 0 | 0 | 1 | 1 | 1 | 32 |
| 5 | 1 | $1/(1 + x)$ | 17 | -1 | QUAD1 | - | -4 | -1 | -2 | -2 | 3.4 |
| 6 | $\sqrt{x}$ | | 57 | -85 | QUAD2 | - | -2 | -1 | -2 | -2 | 17 |
| 7 | $1/\sqrt{x}$ | | [a]137 | -2 | QUAD3 | - | 0 | 0 | 0 | 0 | 27 |
| 8 | $\ln x$ | | [a]109 | +8 | QUAD4 | - | 4 | 5 | 4 | 6 | 22 |
| 9 | $1/\sqrt{x}$ | | [b]157 | -3 | QUAD3 | - | 0 | 0 | 0 | 0 | 31 |
| 10 | $\ln x$ | | [b]117 | -3 | QUAD4 | - | 4 | 5 | 4 | 6 | 23 |
| 11 | 1 | $10e^{-10x}$ | 61 | -7 | QUAD1 | - | - | -65 | -2 | -3 | 7 |
| 12 | $1/\sqrt{x}$ | $\frac{\sqrt{x}\cos x}{2\sqrt{\sin x}}$ | [b]169 | -25 | QUAD3 | 31 | 0 | 0 | -2 | -2 | 34 |
| 13 | 1 | eq. (5) | 98 | - | QUAD1 | - | - | [c]9 | [c]0 | [c]0 | 11 |

(a) $\epsilon = 10^{-4}$.

(b) $\epsilon = 10^{-5}$.

(c) Error relative to SIMPS1.

Example 12 actually represents the integration of

$$\int_0^1 \frac{\cos x}{2\sqrt{\sin x}}\, dx \qquad (6)$$

where there is an implicit $1/\sqrt{x}$ singularity in the integrand. This integral is easily evaluated by QUAD3 when expressed in the form

$$\int_0^1 \frac{\cos x}{2\sqrt{\frac{\sin x}{x}}} \frac{1}{\sqrt{x}}\, dx$$

where the function $\cos x/2\sqrt{\sin x/x}$ is well behaved. Note that this integration does not necessitate a prior evaluation of $\sin x/x$ at $x = 0$ since, as previously mentioned, the Gaussian quadratures do not evaluate the integrand at the end points.

The range of values of the ratio $N_S/N_G$ shown in table II must be considered from two different perspectives: as a measure of the efficiency of Gaussian quadrature methods compared with ordinary Simpson Integration, and as a measure of the Gaussian quadrature methods compared with SIMPS1 (presumably only at Lewis, to date). SIMPS1 is an ingenious function subprogram for the evaluation of integrals wherein the integrand may have many sharp peaks. SIMPS1 does not subdivide the region of integration uniformly, but preferentially subdivides only those subregions where it is necessary to achieve a prescribed maximum error. The basic integration technique employed by SIMPS1 is Simpson's Rule. Hence, SIMPS1, is a Simpson's Rule technique which minimizes the evaluation of the integrand. In other words, to obtain the same accuracy with a normal Simpson's Rule would require evaluation of the integrand at intervals equal to the smallest interval employed by SIMPS1 over the whole range. This would in general, be many times the values shown for $N_S$ in table II for evaluation of the same integrals. Therefore, the ratios $N_S/N_G$ given in table II are very conservative estimates of the efficiency of Gaussian quadrature techniques when compared with ordinary Simpson's Rule.

The ratio $N_S/N_G$ does not provide a fair comparison of the Gaussian quadrature formulas with SIMPS1 since the latter may employ each evaluation of the integrand many times and use many more operations than the former. Table III shows a comparison of three examples from table II on the basis of time. The ratio $T_S/T_G$ shows the increase in speed available with the Gaussian quadrature, where $T_S$ and $T_G$ are the times needed to perform the integration by SIMPS1 and Gaussian quadrature, respectively. In the last column of table III, $T_I$ represents the time spent in evaluating the integrand. Hence, the ratio represents a comparison of the time spent by the two methods in operating on the integrand evaluations.

Table IV gives an indication of the accuracy obtainable with a double precision Gauss' formula (DQUAD1).

TABLE III. - COMPARISON BETWEEN NUMBER OF EVALUATIONS OF INTEGRAND AND COMPUTATION TIME

| Example from table II | Evaluation of integrand | | | Time | |
|---|---|---|---|---|---|
| | $N_S$ | $N_G$ | $N_S/N_G$ | $T_S/T_G$ | $\frac{T_S - T_I}{T_G - T_I}$ |
| 5 | 17 | 5 | 3.4 | 4.7 | 5.3 |
| 9 | 157 | 5 | 31 | 91 | 78 |
| 12 | 169 | 5 | 22 | 46 | 177 |

TABLE IV. - DOUBLE PRECISION EVALUATION OF $\int_0^1 f(x)dx$ BY GAUSS' FORMULA

| f(x) | N | Absolute error |
|---|---|---|
| $\frac{2}{\sqrt{\pi}} e^{-x^2}$ | 16 | $\leq 10^{-15}$ |
| $\cos \frac{5\pi}{2} x$ | 13 | $< 10^{-15}$ |

## CONCLUSIONS

It has been shown that Gaussian quadrature is highly superior to ordinary Simpson's Rule or SIMPS1 for a rather wide class of functions. The examples considered show an increase in actual speed of the Gaussian quadrature routines over SIMPS1 of from 4.7 to 91 times. Since the majority of numerical integrations performed at large computing centers treat far less pathological integrands than those for which SIMPS1 was designed, it would appear advantageous to use the more rapid Gaussian quadratures whenever possible. One advantage of SIMPS1, however, is that it does provide an excellent means of determining the optimum number $N_G$ needed for a given accuracy with Gaussian quadratures.

## APPENDIX - FORTRAN PROGRAM DESCRIPTIONS

### QUAD1/INTEGRATION

**Purpose** Function subprogram used to perform the numerical integration of

$$\int_{XO}^{XF} f(x)\, dx$$

by Gauss' formula. A very powerful method for minimizing machine time in production runs when the integrand and first derivative are continuous in the region of integration.

**Calling Sequence** QUAD1(N,NS,XO,XF,FOFX)
N is the number of points per division.
NS is the number of divisions into which XF-XO is divided (this is provided in case 16 points is not sufficient - see below)
FOFX is an external function subprogram.
N = 3(1)16* 9 D

**Source Language** FORTRAN IV

**Reference** 8

### DQUAD1/DOUBLE PRECISION INTEGRATION

**Purpose** Double Precision version of QUAD1 (q.v.)

**Calling Sequence** DQUAD1(N,NS,XO,XF,FOFX)
FOFX must be a double precision function
N = 3(1)15, 15 D
N = 16(4)24(8)48(16)96, 17 D**

**Reference** 8

*This notation denotes that N takes on all values from 3 to 16 at unit increments; for example, N = 3(1)6(2)12 signifies N = 3,4,5,6,8,10,12.

**Data available to 21 D on punched cards.

## SQUAD1/INTEGRATION OF MULTIPLE INTEGRALS

**Purpose** Subroutine subprogram used to perform the numerical integrations of the types

$$\int_{XO}^{XF} f(x) \int_{ZO(x)}^{ZF(x)} g(x,z)\, dz\, dx$$

by repeated application of Gauss' formula. (cf. QUAD1)

**Calling Sequence**

SQUAD1 (MODE,N,XO,XF,X,Y,ANSWR)
MODE = 1, Obtain arguments X(N).
 = 2, Use evaluations of integrand Y(X(N)) to obtain ANSWR.
N number of points of integration
X arguments - must be dimensioned array name X(N)
Y - must be dimensioned array name Y(N)
ANSWR result of integration

**EXAMPLE**

$$\int_{B}^{C} F(x) \int_{A}^{x} G(x')\, dx'\, dx$$

A,B,C constants
F(X), G(X') function subprograms

```
      -----
      Dimension  XF(NF),YF(NF),XG(NG),YG(NG)
      -----
      CALL SQUAD1 (1,NF,B,C,XF,YF,FINTGL)
      DO  10 I = 1,NF
      CALL SQUAD1 (1,NG,A,XF(I),XG,YG,ANSWR)
      DO 20 J = 1,NG
20    YG(J) = G(XG(J))
      CALL SQUAD1 (2,NG,A,XF(I),XG,YG,ANSWR)
10    YF(I) = ANSWR* F(XF(I))
      CALL SQUAD1 (2,NF,B,C,XF,YF,FINTGL)
      -----
```

## DSQUAD1/DOUBLE PRECISION MULTIPLE INTEGRATION

**Purpose** Double precision version of SQUAD1 (q.v.)

## QUAD2/INTEGRATION

**Purpose** Function subprogram used to perform the numerical integration of

$$\int_{XO}^{XF} \sqrt{|x - XO|}\ f(x)\ dx$$

by weighted Gaussian quadrature. A very powerful technique for minimizing the machine time in production runs when f(x) and its first derivative are continuous throughout the region of integration.

**Calling Sequence** QUAD2(N,XO,XF,FOFX)
See QUAD1
N = 2(1)8     8 D

**Reference** 5

## QUAD3/INTEGRATION

**Purpose** Function subprogram. Used to perform the numerical integration of

$$\int_{XO}^{XF} \frac{f(x)}{\sqrt{|x - XO|}}\ dx$$

by weighted Gaussian quadrature. A very powerful method for minimizing the machine time in production runs when f(x) and its first derivate are continuous throughout the region of integration.

**Calling Sequence** QUAD3(N,XO,XF,FOFX)
See QUAD1
N = 2(1)8(2)12(4)24(8)48     17 D

**Reference** 6

## DQUAD3/DOUBLE PRECISION INTEGRATION

**Purpose** Double precision version of QUAD3 (q.v.)

## QUAD4/INTEGRATION

**Purpose** Function subprogram. Used to perform numerical integration of

$$\int_{XO}^{XF} f(x) \ln |x - XO| \, dx$$

by weighted Gaussian quadrature. A very powerful method for minimizing the machine time in production runs when $f(x)$ and its first derivative are continuous throughout the region of integration.

**Calling Sequence** QUAD4(N,XO,XF,FOFX)
(See QUAD1
N = 3(1)11 9 D

**Method**

$$\int_{XO}^{XF} f(x) \ln |x - XO| \, dx = \Delta X \int_{0}^{1} f(\Delta X \cdot y + XO) \ln y \, dy$$

$$+ \ln |\Delta X| \int_{XO}^{XF} f(x) \, dx$$

where

$$\Delta X = XF - XO$$

$$y \equiv \frac{x - XO}{\Delta X}$$

**Other Subroutines Employed** QUAD1 (q.v.)

**Reference** Private Communication from Peter Sockol

## QUAD5/INTEGRATION

**Purpose**

Function subprogram used to perform the numerical integration of

$$\int_0^{\infty} e^{-x} f(x)\, dx$$

by the Gauss-Laguerre quadrature formula. A very powerful method for minimizing the machine time in production runs when f(x) and its first derivative are continuous throughout the region of integration.

**Calling Sequence**

QUAD5(N,FOFX)
See QUAD1

**Reference**

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## QUAD6/INTEGRATION

**Purpose**

Function subprogram used to perform the numerical integration of

$$\int_{-\infty}^{+\infty} e^{-x^2} f(x)\, dx$$

by the Gauss-Hermite quadrature formula. A very powerful method for minimizing machine times in production runs when f(x) and its first derivative are continuous throughout the range of integration.

**Calling Sequence**

QUAD6(N,FOFX)
See QUAD1

**Reference**

9

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