COMPUTER GENERATION OF QUADRATURE COEFFICIENTS UTILIZING THE SYMBOLIC MANIPULATION LANGUAGE FORMAC

by Paul Swigert

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SUMMARY

A method for constructing quadrature coefficients through the use of a FORMAC computer program is presented. The computer program has the ability to construct exact rational fraction coefficients for quadrature formulas of a wide class of weight functions. Quadrature coefficients, constructed by the FORMAC program, are presented for certain weight functions and collocation points.

INTRODUCTION

Numerical integration of functions is usually easy and straightforward on high-speed computers. This ease, obtained through the use of a general purpose integration subroutine, may be misleading as to efficient programing. The general subroutine must apply an unweighted quadrature formula, such as Simpson's rule, many times over the integration interval to achieve a solution. To keep the error in the solution small some method of testing the accuracy, like differencing, and halving the increment must be incorporated. The very generality of such a program leads to an increase in computer time needed to perform a specific integration. This is especially true if the integrands are not well behaved (e.g., $1/\sqrt{x}$ and $\ln x$). Functions such as these cannot be approximated near the origin by a polynomial and thus cause excessive computer time when being integrated by an unweighted quadrature formula.

A more efficient method of performing numerical integration may be done by quadrature formulas developed specifically for the function to be integrated. The efficiency of a specific quadrature formula over a general purpose integration subroutine increases as the number of integrations to be performed goes up. Thus much computer time may be saved if a single quadrature formula can be used for integrands of a common functional form (e.g., $f(x)\sqrt{x}$).
It can be shown that, if all $x_i$ are independent, the inverse of the Vandermonde matrix may be computed from the following equations:

$$V = LU$$

$$V^{-1} = U^{-1}L^{-1}$$

where $U$ and $L$ are upper and lower triangular matrices, respectively. The elements $u_{ij}$ of $U^{-1}$ are

$$u_{ij} = \begin{cases} 0 & i > j \\ 1 & i = j \\ -u_{1,j-1}x_{j-1} & 1 < j \\ u_{i,j-1} - u_{i-1,j-1} & i < j \end{cases}$$

The elements $l_{ij}$ of $L^{-1}$ are

$$l_{ij} = \begin{cases} 0 & 1 < i < j \\ 1 & i = 1 \\ \frac{1}{\prod_{k=1}^{i-j-1} x_j - x_k} & i \geq j > 1 \\ \prod_{k=1}^{i-j-1} x_j - x_k & k \neq j \end{cases}$$

The final form of the desired matrix equation may now be written

$$HF^T = MU^{-1}L^{-1}F^T$$

The right side of this equation is computed by the FORMAC program described in the following section.
DESCRIPTION OF FORMAC PROGRAM

The function of the FORMAC program is to construct quadrature formulas based on the method described in the preceding section. This computer program, consisting of a main program and an integration subroutine, is written in FORMAC (Formula Manipulation Compiler) for the IBM 7094-7044 direct couple system. FORMAC was chosen as the programming language because of its ability to operate in rational fraction arithmetic and its capability to manipulate mathematical expressions. The former ability allows the calculation of exact quadrature coefficients, while the latter allows for simple input and closed form integration of the various weight functions.

Listings and flow charts of the main program (INTCOF) and the integration subroutine (POLINT) may be found in the appendix. The general flow of the main program and integration subroutine may be obtained from the flow charts. All the matrices and vectors necessary are constructed and manipulated in the main program, while closed form integration, used in construction of the moments of the weight function, is performed in the integration subroutine.

The integration subroutine will integrate, in closed form, any linear combination of the two following functions:

\[ g(x) = \sum_{k=1}^{r} c_k x^{d_k} \]

\[ h(x) = \sum_{k=1}^{s} c_k x^{d_k} \ln x \quad (d_k \neq -1) \]

where \( c_k \) and \( d_k \) are rational constants and \( r \) and \( s \) are positive integers. This subroutine relies on the following indefinite integral formulas:

\[ \int x^{p/q} \, dx = \frac{x^{(p/q)+1}}{p+1} \quad (p/q \neq -1) \]

\[ \int x^{-1} \, dx = \ln x \]
\[ \int x^{p/q} \ln x \, dx = \frac{x^{(p/q)+1}}{p+1} \ln x - \frac{x^{(p/q)+1}}{(p/q + 1)^2} \quad (p/q \neq -1) \]

The result of integration by this subroutine is a symbolic expression for the integral. This integral must, however, be evaluated at the upper and lower limits to determine the moments. This evaluation is performed in the main program.

Since \( \lim_{x \to 0} x \ln x = 0 \), it can be seen that, if the integration range is \((0,1)\) and \(p/q > -1\), irrational numbers will not have to be calculated in any of the integrations. For any other range of integration, it is necessary to keep such quantities as \(2^{1/2}\) and \(\ln 3\), obtained from applying the limits of integration in determining the moments, in their symbolic notation so that exact coefficients may be obtained. This is done automatically in the main program.

**PROGRAM USE**

Input to the quadrature program is entered on two cards. The first card contains the number of collocation points \(n\). This number is in fixed point notation and must end in card column 10. The other input goes in the first 72 card columns of the second card, the order and form of which is shown in table I. Note that the weight function is in terms of a dummy variable \(Z\), that \(\text{FMCLOG}(Z)\) is the FORMAC notation for \(\ln Z\), and that each "piece" of this input is terminated by a dollar sign. Blanks are ignored and may be used freely on this card. The restriction to the first 72 card columns may be altered by changing the READ and DIMENSION statements in the main program. The two examples from table I as they would appear on cards, along with their corresponding output from the program are shown hereinafter.
Certain restrictions are inherent in this program. The specified integration interval and collocation points must be entered as rational fractions. Only weight functions of the type $x^{p/q}$ or $x^{p/q} \log x$ (p/q > -1) are acceptable to the program. Since this program operates in rational arithmetic, the possibility of integer overflow is great. To keep this possibility at a minimum, the integration range should be (0, 1). No more than nine collocation points should be used, and collocation points with large numerators and denominators should be avoided.
DISCUSSION

Quadrature coefficients that have been constructed by this method are presented in table II (pp. 19 and 20). Table II(a) lists the coefficients, $H_i$, for equally spaced collocation points over the closed integration interval $[0, 1]$ and the weight functions $1$, $x^{1/2}$, $x^{-1/2}$, $\ln x$, and $x \ln x$. It might be noted that a linear transformation is all that is needed to transform any finite interval, on the real line, to the interval $[0, 1]$. The coefficients presented, therefore, are applicable to any finite integration interval. The FORMAC program may be used, however, to generate quadrature formulas for other intervals and weight functions.

To give an example of the use of such a linear transformation and to show the use of a quadrature formula from table II(a), suppose a function $F(\xi)$ is to be calculated and is given by

$$F(\xi) = \int_0^\xi \frac{f(t)}{(\xi - t)^{1/2}} dt$$

where $\xi$ is finite and $f(t)$ is not singular in $[0, \xi]$. From the transformation

$$t = \xi (1 - z)$$

the following equations are obtained:

$$dt = -\xi \ dz$$

$$z = \begin{cases} 
1 & \text{when } t = 0 \\
0 & \text{when } t = \xi 
\end{cases}$$

Substituting for $t$ and $dt$ gives

$$F(\xi) = -\xi \int_1^0 \frac{f[\xi (1 - z)]dz}{(\xi - \xi + \xi z)^{1/2}}$$
and, finally,

\[ F(\xi) = \xi^{1/2} \int_0^1 z^{-1/2} f[\xi(1 - z)] \, dz \]

This integral may be readily evaluated by using a quadrature formula with a weight function of \( x^{-1/2} \) from table II(a).

Quadrature coefficients for the same weight functions as those in table II(a) are given in table II(b) for equally spaced points over the half open integration interval \((0, 1]\). This table is useful for integrating functions that have a numerical singularity at the origin. For example, consider the numerical integration of the following:

\[ \int_0^1 \frac{\sqrt{\sin x}}{x} \, dx \]

This may be rewritten as

\[ \int_0^1 \frac{1}{\sqrt{x}} \sqrt{\frac{\sin x}{x}} \, dx \]

At \( x = 0 \), \( (\sin x)/x \) cannot be evaluated on a computer. To handle such an integration, a quadrature formula with a weight function of \( x^{-1/2} \) may be chosen from table II(b). By this method the need to evaluate \( (\sin x)/x \) at \( x = 0 \) is eliminated.

The two examples given previously are only presented to show how the tables can be used. There are, of course, many more applications of the quadrature formulas presented.

In integrating some functions, it may be desirable to place more collocation points in a region of rapid functional change than in other regions. This may be accomplished by specifying the desired points in the program and obtaining a quadrature formula that is specifically designed for the function. This method might also be applied to a function given in tabular form but at nonequidistant points.

Errors resulting from truncation and round off associated with floating point arithmetic have been eliminated from the calculation of these coefficients by the use of FORMAC. To check the errors that can accumulate from floating point round off and truncation, the presented program was run using single precision floating point arithmetic. In five-point quadrature formulas, the errors in the coefficients ranged from
one in the fifth to one in the eighth significant figure. The accuracy could be improved by making use of double precision and better matrix inversion techniques; but the difficult task of determining exactly what the error is in the coefficients would still remain.

A discussion of errors occurring in approximating the integral of a function by a quadrature formula may be found in reference 4. Reference 2 gives exact quadrature coefficients for the weight function $w(x) = x^{-1/2}$ for $n = 2(1)11$ along with an excellent discussion of error bounds on quadrature formulas.

CONCLUDING REMARKS

The calculation of exact quadrature coefficients has been reduced to a FORMAC computer program. This program may easily be used to produce quadrature formulas for a large class of weight functions. The use of quadrature formulas designed for a particular integrand promises to save computer time over the use of a general purpose integration program.

Lewis Research Center,
National Aeronautics and Space Administration,
Cleveland, Ohio, March 29, 1966.
APPENDIX - FORMAC PROGRAM LISTINGS

$IBFMC INTCONF
C FORMAC PROGRAM TO EVALUATE N POINT INTEGRATION
C COEFFICIENTS USING THE VANDERMONDE MATRIX
SYMARG
DIMENSION IX(12,12), IY(12), KY(12), X(12), IN(12), OUT(17)
ATOMIC Y(12), Z, LN1, LN2
LOGICAL KODE
INTEGER QUAD, W, Z, X1, X2, T1, T2
FMCDMP LATER
C READ INPUT
  1 READ (5,101) N, (IN(I), I=1,12)
101 FORMAT (I10/(12A6))
J = 0
LET W = ALGCON IN(1), J
LET X1 = ALGCON IN(1), J
LET X2 = ALGCON IN(1), J
DO 2 I=1, N
  I = I
  LET X(I) = ALGCON IN(1), J
2 CONTINUE
C CONSTRUCT MOMENT VECTOR
DO 10 I=1, N
  I = I
  LET T1 = W*Z**(I-1)
  CALL POLINT(T1, Z, KODE)
  IF(.NOT.KODE) STOP
  LET KY(I) = SUBST T1, (FMCLOG(Z), LN2), (Z*X2)
  LET T1 = SUBST T1, (FMCLOG(Z), LN1), (Z*X1)
  LET KY(I) = EXPAND KY(I) - T1
10 CONTINUE
ERASE T1
C CONSTRUCT LOWER INVERSE
DO 30 I=1, N
  I = I
  DO 30 J=1, N
    J = J
    LET IX(I, J) = 1
    IF(I.GE.J) GO TO 19
    LET IX(I, J) = EXPAND IX(I, J)*(1/(X(I)*X(J)) - X(K))
30 CONTINUE
19 DO 20 K=1, I
  K = K
  IF(K.EQ.J) GO TO 20
  LET IX(I, J) = EXPAND IX(I, J)*(1/(X(J)-X(K)))
20 CONTINUE
C MULTIPLY COLUMN VECTOR BY LOWER INVERSE
DO 40 I=1, N
  I = I
  LET IY(I) = 0
  DO 40 J=1, N
    J = J
    LET IY(I) = EXPAND IY(I) + IX(I, J)*Y(J)
    ERASE IX(I, J)
40 CONTINUE
C CONSTRUCT UPPER INVERSE
LET IX(1,1) = 1
DO 50 J=2, N
  J = J
  LET IX(1, J) = EXPAND IX(1, J-1)*X(J-1)*(-1)
50 CONTINUE
DO 60 I=2,N
    I = I
DO 60 J=1,N
    J = J
    IF(I.LT.J) GO TO 59
    IF(I.EQ.J) GO TO 58
    LET IX(I,J) = 0
    GO TO 60
58 LET IX(I,J) = 1
    GO TO 60
59 LET IX(I,J) = EXPAND IX(I-1,J-1) - IX(I,J-1)*X(J-1)
    CONTINUE
    C MULTIPLY COLUMN VECTOR BY UPPER INVERSE
    DO 70 I=1,N
        I = I
        LET JY(I) = 0
        DO 70 J=1,N
            J = J
            LET JY(I) = EXPAND JY(I) + IX(I,J)*IY(J)
            ERASE IX(I,J)
        70 CONTINUE
    DO 80 I=1,N
        I = I
        ERASE IY(I)
    80 CONTINUE
    C MULTIPLY RESULTING COLUMN VECTOR BY THE MOMENT VECTOR
    LET QUAD = 0
    DO 90 I=1,N
        I = I
        LET QUAD = QUAD + KY(I)*JY(I)
        ERASE KY(I),JY(I)
    90 CONTINUE
    LET QUAD = EXPAND QUAD
    LET T1 = QUAD
    ERASE QUAD
    LET QUAD = 0
    DO 91 I=1,N
        I = I
        LET T2 = COEFF T1*Y(I)
        LET QUAD = QUAD + Y(I)*T2
    91 CONTINUE
    ERASE T1,T2
    LET QUAD = ORDER QUAD,INC,FUL
    LET KODE = FIND QUAD,APP,ONE,(LN1,LN2)
    IF(.NOT.*KODE) GO TO 93
    LET KODE = MATCH ID,X1,1
    IF(.NOT.*KODE) GO TO 92
    LET QUAD = SUBST QUAD,(LN1,0)
    AUTSIM ON
    LET QUAD = SUBST QUAD,(LN2,FMCLOG(X2))
    GO TO 93
92 LET KODE = MATCH ID,X2,1
    IF(.NOT.*KODE) GO TO 94
    LET QUAD = SUBST QUAD,(LN2,0)
    LET KODE = MATCH ID,X1,0
    IF(KODE) GO TO 93
    AUTSIM ON
    LET QUAD = SUBST QUAD,(LN1,FMCLOG(X1))
    GO TO 93
94 AUTSIM ON
    LET QUAD = SUBST QUAD,(LN1,FMCLOG(X1)),(LN2,FMCLOG(X2))
WRITE OUTPUT

93 QUEST = 0.0
LET QUEST = BCDCON W*OUT1,17
WRITE (6,201) (OUT(I),I=2,17)
QUEST = 0.0
LET QUEST = BCDCON X1*OUT1,17
WRITE (6,202) (OUT(I),I=2,17)
QUEST = 0.0
LET QUEST = BCDCON X2*OUT1,17
WRITE (6,203) (OUT(I),I=2,17)
WRITE (6,204)
DO 99 I=1,N
  QUEST = 0.0
  LET QUEST = BCDCON X(I)*OUT1,17
  WRITE (6,205) (OUT(J),J=2,17)
99 CONTINUE
WRITE (6,206) N
QUEST = 0.0
100 LET QUEST = BCDCON QUAD*OUT1,17
WRITE (6,207) (OUT(I),I=2,17)
IF(QUEST.NE.0.0) GO TO 100
ERASE QUAD
AUTSIM QNINT
GO TO 1

201 FORMAT (24H1 THE WEIGHT FUNCTION IS ,16A6)
202 FORMAT (32H1 THE LOWER INTEGRATION LIMIT IS ,16A6)
203 FORMAT (32H1 THE UPPER INTEGRATION LIMIT IS ,16A6)
204 FORMAT (22H1 THE -X- POINTS FOLLOW,///)
205 FORMAT (25X,16A6)
206 FORMAT (5H1 THE ,12,59H POINT INTEGRATION QUADRATURE FOR THE ABOVE *
  CONDITIONS IS -,///)
207 FORMAT (1HK,10X,16A6)
END
Figure 1. Flow chart for main program.
SUBROUTINE POLINT(Y,X,KODE)
C FORMAC SUBROUTINE FOR CERTAIN CLOSED FORM INTEGRATIONS
INTEGER X,Y,Y1,Y2,Y3,Y4,DIV
LOGICAL QUEST,KODE
SYMARG Y,X
ATOMIC X
LET Y = EXPAND X*Y
LET N = CENSUS Y,TERM
LET Y1 =
DO 10 I=1,N
K = 0
IF(I.EQ.N) GO TO 1
LET Y2 = PART Y,M
IF(M.EQ.4) GO TO 1001
FMCDMP NOW
KODE = .FALSE.
RETURN
1 LET Y2 = Y
2 LET QUEST = FIND Y2,APP,ALL,(FMCLDG(X))
   IF(.NOT.QUEST) GO TO 3
   LET Y2 = EXPAND Y2/FMCLDG(X)
   K = 1
3 LET Y3 = Y2
4 LET Y4 = PART Y3,M
   IF(M.NE.1) GO TO 5
   LET Y3 = Y4
   GO TO 4
5 IF(M.NE.5) GO TO 6
   LET QUEST = FIND Y3,APP,ALL,(X)
   IF(QUEST) GO TO 4
   LET Y3 = Y4
   LET QUEST = FIND Y3,APP,ALL,(X)
   IF(QUEST) GO TO 4
   IF(K.EQ.1) GO TO 1001
   LET DIV = Y2*FMCLDG(X)
   GO TO 9
6 IF(M.NE.2) GO TO 7
   IF(K.EQ.0) GO TO 61
   LET DIV = Y2*(FMCLDG(X)-1)
   GO TO 9
61 LET DIV = Y2
   GO TO 9
7 IF(M.NE.3) GO TO 8
   IF(K.EQ.1) GO TO 1001
   LET DIV = Y2*FMCLDG(X)
   GO TO 9
8 IF(K.EQ.0) GO TO 81
   LET DIV = Y2*(FMCLDG(X)/Y3-1/Y3**2)
   GO TO 9
81 LET DIV = Y2/Y3
9 LET Y1 = Y1 + DIV
10 CONTINUE
LET Y = EXPAND Y1
ERASE Y1,Y2,Y3,Y4,DIV
KODE = .TRUE.
RETURN
END
Figure 2. - Flow chart for integration subroutine.
Figure 2. - Concluded.
REFERENCES


TABLE II - QUADRATURE COEFFICIENTS H_i

(a) Closed interval, [0,1]; \( x_i = (i - 1)/(n - 1) \) (i = 1, 2, \cdots, n)

<table>
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<tr>
<th>Weight function, ( w(x) )</th>
<th>Number of collocation points, ( n )</th>
<th>Functional values</th>
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\[ x^{1/2} \]

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\[ x^{-1/2} \]
### Table II. Concluded. Quadrature Coefficients $H_i$

**Half open interval, $(0,1]; \ x_k = i/n \ (i = 1, 2, \ldots, n)$**

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**Note:** The table continues with similar entries for each row and column, providing a comprehensive list of functional values and corresponding coefficients for the quadrature formula.
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—National Aeronautics and Space Act of 1958

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