SUPPLEMENT TO

A Note on the Optimal Addition of Abscissas to Quadrature Formulas of Gauss and Lobatto Type

by

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1         SUBROUTINE KRONRO(N,A,W1,W2,EPS,IER)
      C
      C  THIS SUBROUTINE CALCULATES THE ABSCISSAS A AND WEIGHTS W1
      C  OF THE (2*N+1)-POINT QUADRATURE FORMULA WHICH IS OBTAINED
      C  FROM THE N-POINT GAUSSIAN RULE BY OPTIMAL ADDITION OF
      C  N+1 POINTS. THE OPTIMALLY ADDED POINTS ARE CALLED KRONROD
      C  ABSCISSAS. ABSCISSAS AND WEIGHTS ARE CALCULATED FOR
      C  INTEGRATION ON THE INTERVAL (-1,1). SINCE THIS QUADRATURE
      C  FORMULA IS SYMMETRICAL WITH RESPECT TO THE ORIGINE,ONLY
      C  THE NONNEGATIVE ABSCISSAS ARE CALCULATED. WEIGHTS CORRES-
      C  PONDING TO SYMMETRICAL ABSCISSAS ARE EQUAL.
      C  IN ADDITION, THE WEIGHTS W2 OF THE GAUSSIAN RULE ARE
      C  CALCULATED.
      C
2         REAL*8 A,AK,AN,B,C,TAU,W1,W2,XX
3         DIMENSION A(201),B(201),TAU(201),W1(201),W2(201)
4         COMMON C,INDEKS
      C
      C  INPUTPARAMETERS
      C     N   ORDER OF THE GAUSSIAN QUADRATURE FORMULA TO WHICH
      C         ABSCISSAS MUST BE ADDED.
      C     EPS REQUESTED ABSOLUTE ACCURACY OF THE ABSCISSAS. THE
      C         ITERATIVE PROCESS TERMINATES IF THE ABSOLUTE
      C         DIFFERENCE BETWEEN TWO SUCCESSIVE APPROXIMATIONS
      C         IS LESS THAN EPS.
      C
      C  OUTPUTPARAMETERS
      C     A   VECTOR OF DIMENSION N+1 WHICH CONTAINS THE NONNEGA-
      C         TIVE ABSCISSAS. A(1) IS THE LARGEST ABSCISSA.A(2*K)
      C         IS A GAUSSIAN ABSCISSA.A(2*K-1) IS A KRONROD ABSCISSA.
      C     W1  VECTOR OF DIMENSION N+1 WHICH CONTAINS THE WEIGHTS
      C         CORRESPONDING TO THE ABSCISSAS A.
      C     W2  VECTOR OF DIMENSION N+1, CONTAINING THE GAUSSIAN
      C         WEIGHTS. W2(2*K-1) =0 AND W2(2*K) IS THE GAUSSIAN
      C         WEIGHT CORRESPONDING TO A(2*K).
      C     IER ERROR CODE
      C         IF IER=0  ALL ABSCISSAS ARE FOUND TO WITHIN THE
      C         REQUESTED ACCURACY.
      C         IF IER=1 ONE OF THE ABSCISSAS IS NOT FOUND AFTER
      C         50 ITERATION STEPS AND THE COMPUTATION IS TERMINATED.
      C
      C  REQUIRED SUBPROGRAMS
      C     ABWE1  CALCULATES THE KRONROD ABSCISSAS AND CORRES-
      C            PONDING WEIGHTS.
      C     ABWE2  CALCULATES THE GAUSSIAN ABSCISSAS AND THE COR-
      C            RESPONDING WEIGHTS.
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      C
    5         IER = C
    6         NP = N+1
    7         M = (N+1)/2
    8         INDEKS = 1
    9         IF(2*M.EQ.N) INDEKS=0
   10         D = 2.CDC
   11         AN = C.CDC
   12         DC 1 K=1,N
   13         AN = AN +1.DC
   14       1 D = D*AN/(AN+C.5DC)
   15         DC 2 K=1,NP
   16       2 W2(K) = C.CD+C

   17         N2 = N+N+1
   18         M1 = M-1
      C  CALCULATION CF THE CHEBYSHEV CCEFFICIENTS CF THE CRTHC-
      C  GONAL PCLYNOMIAL.
   19         TAU(1) = (AN+2.DC)/(AN+AN+3.CDO)
   20         B(M) = TAU(1)-1.ODC
   21         IF(N.LT.3) GCTC 4
   22         AK = AN
   23         DC 3 L=1,M1
   24         AK = AK +2.ODO
   25         TAU(L+1) = ((AK-1.CDC)*AK-AN*(AN+1.CDO))*(AK+2.CDO)*TAU(L)/
             1  (AK*((AK+3.CDC)*(AK+2.CDO)-AN*(AN+1.ODO)))
   26         ML = M-L
   27         B(ML) = TAU(L+1)
   28         DC 3 LL=1,L
   29         MM = ML+LL
   30       3 B(ML) = B(ML)+TAU(LL)*B(MM)
   31       4 B(M+1) = 1.ODO
      C  CALCULATION CF APPRCXIMATE VALUES FCR THE ABSCISSAS
   32         BB = SIN(1.57C796/(SNGL(AN+AN)+1.))
   33         X = SQRT(1.-BB*BB)
   34         S = 2.*BB*X
   35         C = SQRT(1.-S*S)
   36         CCEF = 1.-(1.-1./AN)/(8.*AN*AN)
   37         XX = CCEF*X
   38         DC 5 K=1,N,2
      C  CALCULATION CF THE K-TH ABSCISSA (=KRCNRCD ABSCISSA) AND
      C  THE CCRRESPONDING WEIGHT.
   39         CALL ABWE1(XX,B,M,EPS,W1(K),N,IER)
   40         IF(IER.EQ.1) RETURN
   41         A(K) = XX
   42         Y = X
   43         X = Y*C-BB*S
   44         BB = Y*S+BB*C
   45         XX = CCEF*X
   46         IF(K.EQ.N) XX = C.CDO
      C  CALCULATION CF THE (K+1)-TH ABSCISSA (=GAUSSIAN ABSCISSA)
      C  AND THE CCRRESPONDING WEIGHTS.
   47         CALL ABWE2(XX,B,M,EPS,W1(K+1),W2(K+1),N,IER)
   48         IF(IER.EQ.1) RETURN
   49         A(K+1) = XX
   50         Y = X
   51         X = Y*C-BB*S
   52         BB = Y*S+BB*C
   53       5 XX = CCEF*X
   54         IF(INDEKS.EQ.1) GCTC 6
   55         A(N+1) = C.ODC
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      CALL ABWE1(A(N+1),B,M,EPS,W1(N+1),N,IER)
    6 RETURN
      END

      SUBROUTINE ABWE1(X,A,N,EPS,W,N1,IER)
      REAL*8 A,AI,B0,B1,B2,COEF,C0,C1,C2,DELTA,F,FD,W,X,YY
      DIMENSION A(201)
      COMMON COEF,INDEKS
      ITER = 0
      KA = 0
      IF(X.EQ.0.0D0) KA=1
    1 ITER = ITER+1
C  START ITERATIVE PROCESS FOR THE COMPUTATION OF A KRONROD
C  ABSCISSA.
C  TEST ON THE NUMBER OF ITERATION STEPS
      IF(ITER.LT.50) GOTO 2
      IER = 1
      RETURN
    2 B1 = 0.0D0
      B2 = A(N+1)
      YY = 4.0D0*X*X-2.0D0
      D1 = 0.0D0
      IF(INDEKS.EQ.1) GOTO 3
      AI = N+N+1
      D2 = AI*A(N+1)
      DIF = 2.0D0
      GOTO 4
    3 AI = N+1
      D2 = 0.0D0
      DIF = 1.0D0
    4 DO 5 K=1,N
      AI = AI-DIF
      I = N-K+1
      B0 = B1
      B1 = B2
      D0 = D1
      D1 = D2
      B2 = YY*B1-B0+A(I)
      I = I+INDEKS
    5 D2 = YY*D1-D0+AI*A(I)
      IF(INDEKS.EQ.1) GOTO 6
      F = X*(B2-B1)
      FD = D2+D1
      GOTO 7
    6 F = 0.5D0*(B2-B0)
      FD = 4.0D0*X*D2
    7 DELTA = F/FD
      X = X-DELTA
      IF(KA.EQ.1) GOTO 8
C  TEST ON CONVERGENCE.
      IF(DABS(DELTA).GT.EPS) GOTO 1
      KA = 1
      GOTO 1
C  COMPUTATION OF THE WEIGHT.
    8 D0 = 1.0D0
      D1 = X
      AI = 0.0D+0
      DO 9 K=2,N1
      AI = AI+1.0D+0
      D2 = ((AI+AI+1.0D+0)*X*D1-AI*D0)/(AI+1.0D+0)
      D0 = D1
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111       5    D1 = D2
112            W = COEF/(FD*D2)
113            RETURN
114            END

115            SUBROUTINE ABWE2(X,A,N,EPS,W1,W2,N1,IER)
116            REAL*8 A,AN,COEF,DELTA,PO,P1,P2,PDO,PD1,PD2,W1,W2,X,YY
117            DIMENSION A(2C1)
118            COMMON COEF,INDEKS
119            ITER = C
120            KA = C
121            IF(X.EQ.C.CDC) KA=1
       C   START ITERATIVE PROCESS FOR THE COMPUTATION OF A GAUSSIAN
       C   ABSCISSA.
122       1    ITER = ITER+1
       C   TEST ON THE NUMBER OF ITERATION STEPS.
123            IF(ITER.LT.5O) GOTO 2
124            IER = 1
125            RETURN
126       2    PO = 1.DO
127            P1 = X
128            PDO = C.DO
129            PD1 = 1.OD+0
130            AI = C.OD+C
131            DO 3 K=2,N1
132            AI = AI+1.DO
133            P2 = ((AI+AI+1.DO)*X*P1-AI*PO)/(AI+1.DO)
134            PD2 = ((AI+AI+1.D+C)*(P1+X*PD1)-AI*PDO)/(AI+1.DO)
135            PO = P1
136            P1 = P2
137            PDO = PD1
138       3    PD1 = PD2
139            DELTA = P2/PD2
140            X = X-DELTA
141            IF(KA.EQ.1) GOTO 4
       C   TEST ON CONVERGENCE.
142            IF(DABS(DELTA).GT.EPS) GOTO 1
143            KA = 1
144            GOTO 1
145       4    AN = N1
       C   COMPUTATION OF THE GAUSSIAN WEIGHT.
146            W2 = 2.DO/(AN*PD2*PO)
147            P1 = C.DDC
148            P2 = A(N+1)
149            YY = 4.CDC*X*X-2.DC
150            DO 5 K=1,N
151            I = N-K+1
152            PO = P1
153            P1 = P2
154       5    P2 = YY*P1-PO+A(I)
155            IF(INDEKS.EQ.1) GOTO 6
       C   COMPUTATION OF THE OTHER WEIGHT.
156            W1 = COEF/(PD2*X*(P2-P1))+W2
157            GOTO 7
158       6    W1 = 2.DO*COEF/(PD2*(P2-PO))+W2
159       7    RETURN
160            END
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