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

By Robert Piessens and Maria Branders

Abstract. An improved method for the optimal addition of abscissas to quadrature formulas of Gauss and Lobatto type is given.

1. Introduction. We consider the quadrature formula

$$\int_{-1}^{+1} f(x)\,dx \simeq \sum_{k=1}^{N} \alpha_k f(x_k) + \sum_{k=1}^{N+1} \beta_k f(\xi_k), \tag{1}$$

where the x_k's are the abscissas of the N-point Gaussian quadrature formula. We want to determine the additional abscissas ξ_k and the weights α_k and β_k so that the degree of exactness of (1) is maximal. This problem has already been discussed by Kronrod [1] and Patterson [2] and it is well known that the abscissas ξ_k must be the zeros of the polynomial $\phi_{N+1}(x)$ which satisfies

$$\int_{-1}^{+1} P_N(x)\phi_{N+1}(x)x^k\,dx = 0, \qquad k = 0, 1, \cdots, N, \tag{2}$$

where $P_N(x)$ is the Legendre polynomial of degree N. Thus, $\phi_{N+1}(x)$ must be an orthogonal polynomial with respect to the weight function $P_N(x)$. Then, the weights α_k and β_k can be determined so that the degree of exactness of (1) is $3N + 1$ if N is even and $3N + 2$ if N is odd.

Szegö [3] proved that the zeros of $\phi_{N+1}(x)$ and $P_N(x)$ are distinct and alternate on the interval $[-1, +1]$. Kronrod [1] gave a simple method for the computation of the coefficients of $\phi_{N+1}(x)$. This method requires the solution of a triangular system of linear equations, which is, unfortunately, very ill-conditioned. Patterson [2] expanded $\phi_{N+1}(x)$ in terms of Legendre polynomials. The coefficients of this expansion satisfy a linear system of equations which is well-conditioned, although its construction requires a certain amount of computing time.

The present note proposes the expansion of $\phi_{N+1}(x)$ in a series of Chebyshev polynomials. We also give explicit formulas for the weights α_k and β_k. Finally, we consider the optimal addition of abscissas to Lobatto rules. As compared with Patterson's method, our method has three advantages:

(i) It leads to a considerable saving in computing time since the formulas are much simpler.

(ii) The loss of significant figures through cancellation and round-off is slightly reduced, as we verified experimentally. This is in agreement with some theoretical results given by Gautschi [4].

(iii) It is applicable for every value of N, while Patterson's method fails in the

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Lobatto case for $N = 7, 9, 17, 22, 27, 35, 36, 37, 40, \cdots$, since some of the denominators in his recurrence formulae become zero.

2. Optimal Addition of Abscissas to Gaussian Quadrature Formulas. It is evident that $\phi_{N+1}(x)$ is an odd or even function depending on whether N is even or odd. Thus, $\phi_{N+1}(x)$ can be expressed as

$$\phi_{N+1}(x) = \sum_{k=0}^{m}{}' b_k T_{2k}(x), \quad \text{if } N \text{ is odd,} \tag{3}$$

and

$$\phi_{N+1}(x) = \sum_{k=0}^{m} b_k T_{2k+1}(x), \quad \text{if } N \text{ is even,} \tag{4}$$

where $m = [(N + 1)/2]$.

It is clear that the polynomial $\phi_{N+1}(x)$ is only defined to within an arbitrary multiplicative constant. For the sake of convenience, we assume $b_m = 1$.

From (2), we derive the condition

$$\int_{-1}^{+1} P_N(x)\phi_{N+1}(x)T_k(x)\,dx = 0, \qquad k = 0, 1, \cdots, N. \tag{5}$$

In order to calculate the coefficients b_k, $k = 0, 1, \cdots, m - 1$, (3) or (4) is substituted in (5). This leads to the system of equations

$$\begin{aligned} b_{m-1} &= \tau_1 - 1, \\ b_{m-k} &= \sum_{j=1}^{k-1} b_{m-k+j}\tau_j + \tau_k, \qquad k = 2, 3, \cdots, m, \end{aligned} \tag{6}$$

where

$$\tau_k = -\int_{-1}^{+1} P_N(x)T_{N+2k}(x)\,dx \bigg/ \int_{-1}^{+1} P_N(x)T_N(x)\,dx. \tag{7}$$

In order to derive a recurrence formula for τ_k, we consider the integral

$$J = \int_{-1}^{+1} [xP_N(x) - P_{N+1}(x)]T_l(x)\,dx. \tag{8}$$

Using a well-known property of the Chebyshev polynomials, we obtain

$$J = \frac{1}{2}\int_{-1}^{+1} [xP_N - P_{N+1}]\, d\left(\frac{T_{l+1}}{l+1} - \frac{T_{l-1}}{l-1}\right), \tag{9}$$

and, by integrating by parts, this integral can be expressed as

$$J = \frac{N}{2(l+1)} I_{N,l+1} - \frac{N}{2(l-1)} I_{N,l-1}, \tag{10}$$

where

$$I_{N,l} = \int_{-1}^{+1} P_N(x)T_l(x)\,dx. \tag{11}$$

On the other hand, using a property of the Legendre polynomials, (8) can be transformed into

$$J = \frac{1}{N+1} \int_{-1}^{+1} (1 - x^2) T_l(x)\, d(P_N(x)),$$

which can be expressed as

$$(12) \qquad J = \frac{2+l}{2(N+1)} I_{N,l+1} + \frac{2-l}{2(N+1)} I_{N,l-1}.$$

Since $\tau_k = I_{N,N+2k}/I_{N,N}$, the recurrence formula

$$(13) \qquad \tau_{k+1} = \frac{[(N+2k-1)(N+2k) - (N+1)N](N+2k+2)}{[(N+2k+3)(N+2k+2) - (N+1)N](N+2k)} \tau_k,$$

where $\tau_1 = (N+2)/(2N+3)$ can be easily derived from (10) and (12).

System (6) is easier to construct than the corresponding system of Patterson [2], inasmuch as his method requires a set of recursions of variable lengths, while in our method only one recursion is needed. Moreover, further economy is achieved in solving the equation $\phi_{N+1}(x) = 0$, since, using a modification of Clenshaw's algorithm of summation, an odd or even Chebyshev series can be evaluated more efficiently than an odd or even Legendre series [5, p. 10]. Indeed, the computing time can be halved.

Explicit formulas for the weights are

$$(14) \qquad \alpha_k = \frac{C_N}{P_N'(x_k)\phi_{N+1}(x_k)} + \frac{2}{NP_{N-1}(x_k)P_N'(x_k)}, \qquad k = 1, 2, \cdots, N,$$

$$(15) \qquad \beta_k = \frac{C_N}{\phi_{N+1}'(\xi_k)P_N(\xi_k)}, \qquad k = 1, 2, \cdots, N+1,$$

where $C_N = 2^{2N+1}(N!)^2/(2N+1)!$.

3. Optimal Addition of Abscissas to Lobatto Quadrature Formulas. We now consider the quadrature formula

$$(16) \qquad \int_{-1}^{+1} f(x)\, dx \simeq \sum_{k=0}^{N+1} \alpha_k f(x_k) + \sum_{k=1}^{N+1} \beta_k f(\xi_k),$$

where the x_k's are abscissas of the Lobatto quadrature formula. Consequently, $x_0 = -1$, $x_{N+1} = +1$ and $x_1, x_2, \cdots, x_N$ are the zeros of the Jacobi polynomial $P_N{}^{(1,1)}(x)$. It is our purpose to determine the free abscissas ξ_k and the weights α_k and β_k so that the degree of exactness of (16) is maximal. Then, ξ_k must be a zero of the polynomial $\phi_{N+1}(x)$ which satisfies

$$(17) \qquad \int_{-1}^{+1} (1 - x^2) P_N^{(1,1)}(x) \phi_{N+1}(x) T_k(x)\, dx = 0, \qquad k = 0, 1, 2, \cdots, N.$$

Again, we express $\phi_{N+1}(x)$ in terms of Chebyshev polynomials as in (3) or (4), according to the parity of N. The coefficients b_k can be found by solving the system (6) where

$$(18) \qquad \tau_k = -\int_{-1}^{+1} (1 - x^2) P_N^{(1,1)} T_{N+2k}\, dx \Big/ \int_{-1}^{+1} (1 - x^2) P_N^{(1,1)} T_N\, dx.$$

Using the relation

$$\int_{-1}^{+1} (1 - x^2) P_N^{(1,1)} T_l \, dx = \frac{1}{N+2} [(l+2) I_{N+1,l+1} - (l-2) I_{N+1,l-1}],$$

where $I_{N,l}$ is defined by (11), the recurrence formula

$$(19) \quad \tau_{k+1} = \frac{[(N+2k-1)(N+2k-2) - (N+1)(N+2)](N+2k+2)}{[(N+2k+3)(N+2k+4) - (N+1)(N+2)](N+2k)} \tau_k$$

can be derived from (13).

The starting value for (19) is

$$\tau_1 = 3(N+2)/(2N+5).$$

The expressions for the weights are

$$(20) \quad \alpha_k = \frac{C_N}{2P_N'(x_k)\phi_{N+1}(x_k)} + \frac{2}{(N+1)(N+2)[P_{N+1}(x_k)]^2}, \qquad \text{for } k = 1, 2, \cdots, N,$$

$$(21) \quad \alpha_0 = \alpha_{N+1} = \frac{2}{(N+2)(N+1)} - \frac{C_N}{2(N+1)\phi_{N+1}(1)},$$

$$(22) \quad \beta_k = \frac{N+2}{2(N+1)} \frac{C_N}{[P_N(\xi_k) - \xi_k P_{N+1}(\xi_k)]\phi_{N+1}'(\xi_k)}, \qquad k = 1, 2, \cdots, N+1,$$

where $C_N = 2^{2N+3}[(N+1)!]^2/(2N+3)!$.

Appendix. Computer program. In this appendix, we describe a FORTRAN program for the construction of the quadrature formula (1). A listing of this program is reproduced in the supplement at the end of this issue. A program for the construction of the quadrature formula (11) may be obtained from the authors.

The program consists of three subroutines: the main subroutine KRONRO and two auxiliary subroutines ABWE1 and ABWE2, which are called by KRONRO.

In KRONRO the coefficients of the polynomial $\phi_{N+1}(x)$ are calculated.

In ABWE1 the abscissas x_k and weights α_k are calculated.

In ABWE2 the abscissas ξ_k and weights β_k are calculated.

The abscissas are calculated using Newton-Raphson's method. Starting values for this iterative process are provided by [6]

$$x_k \simeq \left(1 - \frac{1}{8N^2} + \frac{1}{8N^3}\right) \cos\left(\frac{2k - 1/2}{2N+1} \pi\right)$$

and

$$\xi_k \simeq \left(1 - \frac{1}{8N^2} + \frac{1}{8N^3}\right) \cos\left(\frac{2k - 3/2}{2N+1} \pi\right).$$

The program has been tested on the computer IBM 370/155 of the Computing Centre of the University of Leuven, for $N = 2(1)50(10)200$. The computations were carried out in double precision (approximately 16 significant figures). For $N = 200$, the maximal absolute error of the abscissas is 8.6×10^{-16} and of the weights 3.3×10^{-15}.

For $N = 50$, the computing time is 1.7 sec., for $N = 100$, 6.4 sec. and for $N = 200$, 24.7 sec.

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SUPPLEMENT TO

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by

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pp. 135-139, this issue

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1          SLBRCLTINE KRONRC(N,A,h1,h2,EPS,IER)
      C
      C  TFIS SLBRCLTINE CALCLLATES THE ABSCISSAS A ANC WEIGHTS W1
      C  CF THE (2*N+1)-POINT CUACRATURE FORMULA WHICF IS OBTAINEC
      C  FRCM TFE N-PCINT GALSSIAN RULE BY OPTIMAL ACCITION OF
      C  N+1 PCINTS. THE CPTIMALLY ACCED POINTS ARE CALLEC KRCNROC
      C  ABSCISSAS. ABSCISSAS ANC hEIGHTS ARE CALCULATEC FCR
      C  INTEGRATICN CN THE INTERVAL (-1,1). SINCE THIS QUACRATURE
      C  FCRMLLA IS SYMMETRICAL hITF RESPECT TO TFE CRIGINE,CNLY
      C  TFE NCNNEGATIVE ABSCISSAS ARE CALCULATEC. WEIGFTS CORRES-
      C  PCNCING TC SYMMETRICAL ABSCISSAS ARE ECLAL.
      C  IN ACCITION, THE WEIGFTS h2 CF THE GAUSSIAN RULE ARE
      C  CALCLLATEC.
      C
2          REAL*E A,AK,AN,B,C,TAL,h1,h2,XX
3          CIMENSICN A(2C1),B(201),TAU(201),W1(201),h2(2C1)
4          CCMMCN C,INDEKS
      C
      C  INPLTPARAMETERS
      C     N    CRCER OF THE GALSSIAN CUACRATURE FCRMULA TO WHICF
      C          ABSCISSAS MUST BE ACCEC.
      C     EPS  RECLESTED ABSCLUTE ACCURACY OF THE ABSCISSAS. THE
      C          ITERATIVE PRCCESS TERMINATES IF TFE ABSCLUTE
      C          CIFFERENCE BEThEEN ThO SUCCESSIVE APPRCXIMATIONS
      C          IS LESS THAN EPS.
      C
      C  CLTPLTPARAMETERS
      C     A    VECTCR OF CIMENSICN N+1 WFICH CCNTAINS THE NONNEGA-
      C          TIVE ABSCISSAS. A(1) IS TFE LARGEST ABSCISSA.A(2*K)
      C          IS A GAUSSIAN ABSCISSA.A(2*K-1) IS A KRCNRCC ABSCISSA.
      C     h1   VECTCR CF DIMENSICN N+1 hFICH CCNTAINS THE hEIGFTS
      C          CCRRESPONDING TC THE ABSCISSAS A.
      C     h2   VECTCR OF CIMENSICN N+1, CONTAINING TFE GAUSSIAN
      C          hEIGHTS. h2(2*K-1) =C AND W2(2*K) IS THE GAUSSIAN
      C          hEIGHT CCRRESPCNCING TC A(2*K).
      C     IER  ERRCR CODE
      C          IF IER=0  ALL ABSCISSAS ARE FCUNC TC hITHIN TFE
      C          REQLESTED ACCLRACY.
      C          IF IER=1 ONE CF TFE ABSCISSAS IS NCT FCLNC AFTER
      C          5C ITERATICN STEPS ANC THE CCMPLTATION IS TERMINATEC.
      C
      C  RECLIREC SLBPROGRAMS
      C     ABhE1  CALCULATES TFE KRCNRCD ABSCISSAS ANC CCRRES-
      C            PONCING hEIGHTS.
      C     ABhE2  CALCULATES TFE GALSSIAN ABSCISSAS ANC TFE CCR-
      C            RESPONDING hEIGHTS.
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```
C
      IER = 0
      NP = N+1
      M = (N+1)/2
      INDEKS = 1
      IF(2*M.EQ.N) INDEKS=0
      D = 2.0D0
      AN = 0.0D0
      DO 1 K=1,N
      AN = AN +1.D0
    1 D = D*AN/(AN+0.5D0)
      DO 2 K=1,NP
    2 W2(K) = 0.0D+D

      N2 = N+N+1
      M1 = M-1
C  CALCULATION OF THE CHEBYSHEV COEFFICIENTS OF THE ORTHO-
C  GONAL POLYNOMIAL.
      TAU(1) = (AN+2.D0)/(AN+AN+3.D0)
      B(M) = TAU(1)-1.0D0
      IF(N.LT.3) GOTO 4
      AK = AN
      DO 3 L=1,M1
      AK = AK +2.0D0
      TAU(L+1) = ((AK-1.0D0)*AK-AN*(AN+1.0D0))*(AK+2.0D0)*TAU(L)/
     1 (AK*((AK+3.0D0)*(AK+2.0D0)-AN*(AN+1.0D0)))
      ML = M-L
      B(ML) = TAU(L+1)
      DO 3 LL=1,L
      MM = ML+LL
    3 B(ML) = B(ML)+TAU(LL)*B(MM)
    4 B(M+1) = 1.0D0
C  CALCULATION OF APPROXIMATE VALUES FOR THE ABSCISSAS
      BB = SIN(1.570796/(SNGL(AN+AN)+1.))
      X = SQRT(1.-BB*BB)
      S = 2.*BB*X
      C = SQRT(1.-S*S)
      COEF = 1.-(1.-1./AN)/(8.*AN*AN)
      XX = COEF*X
      DO 5 K=1,N,2
C  CALCULATION OF THE K-TH ABSCISSA (=KRONROD ABSCISSA) AND
C  THE CORRESPONDING WEIGHT.
      CALL ABWE1(XX,B,M,EPS,W1(K),N,IER)
      IF(IER.EQ.1) RETURN
      A(K) = XX
      Y = X
      X = Y*C-BB*S
      BB = Y*S+BB*C
      XX = COEF*X
      IF(K.EQ.N) XX = 0.0D0
C  CALCULATION OF THE (K+1)-TH ABSCISSA (=GAUSSIAN ABSCISSA)
C  AND THE CORRESPONDING WEIGHTS.
      CALL ABWE2(XX,B,M,EPS,W1(K+1),W2(K+1),N,IER)
      IF(IER.EQ.1) RETURN
      A(K+1) = XX
      Y = X
      X = Y*C-BB*S
      BB = Y*S+BB*C
    5 XX = COEF*X
      IF(INDEKS.EQ.1) GOTO 6
      A(N+1) = 0.0D0
      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,D0,D1,D2,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.D0
      GOTO 4
    3 AI = N+1
      D2 = 0.0D0
      DIF = 1.D0
    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.D0*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.D0
      D1 = X
      AI = 0.D+0
      DO 9 K=2,N1
      AI = AI+1.D+0
      D2 = ((AI+AI+1.D+0)*X*D1-AI*D0)/(AI+1.D+0)
      D0 = D1
    9   C1 = C2
        W = CCEF/(FD*C2)
        RETLRN
        ENC

        SLBRCLTINE ABWE2(X,A,N,EPS,W1,W2,N1,IER)
        REAL*8 A,AN,CCEF,CELTA,PC,P1,P2,PDO,PC1,PC2,W1,W2,X,YY
        CIMENSICN A(2C1)
        COMMCN COEF,INDEKS
        ITER = C
        KA = C
        IF(X.EQ.C.CDC) KA=1
  C  START ITERATIVE PROCESS FCR THE CCMPUTATICN CF A GAUSSIAN
  C  ABSCISSA.
    1   ITER = ITER+1
  C  TEST CN THE NUMBER CF ITERATICN STEPS.
        IF(ITER.LT.5C) GCTC 2
        IER = 1
        RETURN
    2   PC = 1.CC
        P1 = X
        PCC = C.DC
        PC1 = 1.CC+0
        AI = C.CD+C
        DC 3 K=2,N1
        AI = AI+1.DO
        P2 = ((AI+AI+1.CC)*X*P1-AI*PO)/(AI+1.CO)
        PC2 = ((AI+AI+1.C+C)*(P1+X*PC1)-AI*PCO)/(AI+1.CO)
        PC = P1
        P1 = P2
        PCC = PC1
    3   PC1 = PC2
        CELTA = P2/PC2
        X = X-DELTA
        IF(KA.EQ.1) GCTC 4
  C  TEST CN CCNVERGENCE.
        IF(CABS(CELTA).GT.EPS) GCTC 1
        KA = 1
        GCTC 1
    4   AN = N1
  C  CCMPLTATICN CF THE GALSSIAN WEIGHT.
        W2 = 2.DO/(AN*PD2*PC)
        P1 = C.CDC
        P2 = A(N+1)
        YY = 4.CDC*X*X-2.CC
        DC 5 K=1,N
        I = N-K+1
        PC = P1
        P1 = P2
    5   P2 = YY*P1-PO+A(I)
        IF(INCEKS.EQ.1) GCTC 6
  C  CCMPUTATICN CF THE CTHER WEIGHT.
        W1 = CCEF/(PC2*X*(P2-P1))+W2
        GCTC 7
    6   W1 = 2.CO*COEF/(PC2*(P2-PO))+W2
    7   RETLRN
        ENC
```