Discrete group symmetry in the fast Chebyshev transform

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Abstract

We consider nonadaptive Clenshaw-Curtis (CC) quadrature of variable degree $n = 2^m, m = 2, 3, \cdots$. The computation of the coefficients of the truncated Chebyshev series expansion of the integrand is shown to be done accurately and efficiently within a fast Chebyshev algorithm. It takes into account the binary tree structures with heap ordering key of the coefficients, the splitting of the $n \times n$ coefficient matrix into irreducible $2^l \times 2^l$ blocks, where l denotes the depth level of the children inside the heap, and the group symmetry properties which can be defined inside each block.

1 Introduction

The computation of the Riemann definite integral

$$I = \int_a^b g(x) f(x) dx, \ -\infty < a < b < \infty, \tag{1}$$

by means of Clenshaw-Curtis (CC) quadrature sums [1] or their extensions (ECC) to oscillatory or hyperbolic weight functions [2], [3], [4] covers the most

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important numerical problems involving observables which relate variables from the direct and the reciprocal spaces.

A CC quadrature sum interpolates the reduced integrand

$$\phi(y) = f(c + hy),\ c = (b + a)/2,\ h = (b - a)/2\ ,\ y \in [-1, 1], \qquad (2)$$

at the CC quadrature abscissas

$$\{y_{n,j} = \cos(j\pi/n) | j = 0, 1...n\}, \qquad (3)$$

by the truncated Chebyshev series expansion

$$L_n^{\phi}(y) = \sum_{k=0}^{n}{}'' b_{n,k} T_k(y), \qquad (4)$$

where the double prime shows that the first and the last terms of the sum are halved.

From the numerical point of view, the use of (4) for the approximation of the reduced integrand $\phi(y)$ (assumed to be a Lipschitz function) shows the advantage that such an expansion is close to the minimax polynomial approximation: the deviations of the interpolatory polynomial $L_n^{\phi}(y)$ from the values of $\phi(y)$ inbetween the quadrature abscissas (3) remain *finite* as $n \to \infty$, and hence the output reliability is substantially increased over other kinds of quadrature rules (like the highest polynomial degree precision Gauss quadrature which uses least squares polynomial expansions).

The computation of the column vector

$$B = (n/2)(b_{n,0}, \cdots, b_{n,n})^{\top} \qquad (5)$$

in the expansion (4) involves the matrix product

$$B = TF, \qquad (6)$$

with a symmetric T matrix, $T_{kj} = T_{jk}$, where

$$T_{kj} = T_k(y_{n,j}),\ k, j = 0, 1, \cdots, n; \qquad F = (f(x_{n,0}), \cdots, f(x_{n,n}))^{\top}. \qquad (7)$$

Gentleman [5] was the first to note that the computation of the coefficients of the expansion (4) within CC quadrature can take advantage of the fast Fourier technique (FFT) to avoid the well-known multiplication bottleneck which limits the efficiency of the computation of (6) at large n. However, only solutions concerning particular finite n values of the polynomial degree have been reported so far.

In the present paper, a fast Chebyshev transform (FCT) algorithm for the computation of (6) is discussed for expansion degrees $n = 2^m,\ m \in \mathbf{N}^+$. The discussion is conveniently divided into three parts: efficient and accurate computation of CC abscissa sets (section 2), irreducible block decomposition of the T matrix (section 3), and symmetry properties inside the blocks (section 4). The paper ends with conclusions in section 5.

2 Computation of CC abscissa sets

In Eq. (3), the quadrature abscissas are labeled in *increasing order of the arguments* of the cosine function. The values of the quadrature abscissas themselves *monotonically decrease* from $y_{n,0} = 1$ to $y_{n,n} = -1$ such that

$$y_{n,n-j} = -y_{n,j}. \tag{8}$$

Under *even* n, the middle abscissa $y_{n,n/2} = 0$. These properties show that, for $n = 2^m$, there are $2^{m-1} - 1$ nontrivial abscissas of the set (3) lying inside the open interval $(0, 1)$.

Within the variable degree nonadaptive quadrature, the accuracy of the quadrature sums approximating the integral (1) is increased by successively doubling the degree n of the interpolatory polynomial (4). Under such an operation, the CC quadrature abscissas (3) show the property of *inheritance*,

$$y_{2n,2j} = y_{n,j}, \tag{9}$$

such that, at $n = 2^m, m \geq 2$, the number of *newly added* abscissas for the implementation of the CC quadrature sums at the doubled current degree n equals 2^{m-2} inside $(0, 1)$. These abscissas cover the *odd label* values

$$y_{2^m,2j-1} = \cos[(2j-1)\pi/2^m], \quad j = 1, 2, \cdots, 2^{m-2}. \tag{10}$$

Due to this property, the sets of odd label abscissas generated at successive degrees $n = 2^m, m \geq 2$ *define a binary tree* having the root $y_{4,1}$.The $2^l, l = 1, 2, \cdots$, newly generated abscissas at degrees $n = 8, 16, \cdots$, are placed at the l-th depth level inside the tree. We associate to this tree a heap ordering key which, for the sake of easy implementation of an iterative computer code, orders the siblings inside a given depth level l in *increasing order of* *the arguments* in the set (10). In what follows the binary tree and its heap ordering key generated at given m will be referred to as H_m.

Although the expressions (10) of the elements of the tree involve trigonometric functions, the occurrence of special arguments allows their computation to machine accuracy over all the tree depth of interest using square root and recurrence.

Indeed, for the root tree we have $y_{4,1} = \sqrt{2}/2$.

To compute the descendants at the $(l+1)$-th level, let us consider a father at the l-th level. Let 2α denote the argument of father's abscissa in (10). We can associate it two "genetic descendants", of arguments α and $\pi/2 - \alpha$ respectively. We have

$$\cos(\alpha) = \sqrt{[\tfrac{1}{2}\cos(2\alpha) + \tfrac{1}{2}]}\ ; \tag{11}$$

$$\cos(\pi/2 - \alpha) = \sin(\alpha) = \frac{\sin(2\alpha)}{2\cos(\alpha)}. \tag{12}$$

The equation (11) computes the value of the *left descendant* $(\cos\alpha)$ based on the value of the reference father $(\cos 2\alpha)$. The equation (12) computes the value of the *right descendant* based on the value of the "genetically related sibling of the reference father" $(\sin 2\alpha)$ and the value of the just computed left descendant $(\cos\alpha)$ which is the genetically related sibling of the right descendant.

3 T matrix irreducible block decomposition

Within the variable degree nonadaptive CC quadrature, the information already acquired at the polynomial degree $2^{m-1} (m \geq 2)$ is preserved if this degree is doubled to 2^m. The most efficient implementation of CC quadrature sums will therefore make use of the values $b_{2^{m-1},q}$ of the already computed coefficients of truncated Chebyshev series expansion. A way to achieve this aim is to make use of the recurrence relations satisfied by the Chebyshev coefficients of (6), namely,

$$B_{2^m,q} = B_{2^{m-1},q} + C_{2^m,q}, \tag{13}$$

$$B_{2^m,2^m-q} = B_{2^{m-1},q} - C_{2^m,q}, \quad q = 0, 1, \cdots, 2^{m-1} - 1, \tag{14}$$

$$B_{2^m,2^{m-1}} = B_{2^{m-1},2^{m-1}}. \tag{15}$$

Irreducible expressions of the corrections $C_{2^m,q}$ are established by complete induction,

$$\begin{aligned} C_{2^m,\,2^s(2p-1)} &= \sum_{i=1}^{2^{m-(s+2)}} T_{2p-1}(y_{2^{m-s},\,2i-1})\delta_{s+1}(2i-1), & (16)\\ & \quad s=0,1,\cdots,m-2, \quad p=1,2,\cdots,2^{m-(s+2)}, \quad m\geq 2. \\ C_{2^m,\,0} &= \sigma_{m-1}(1), & (17) \end{aligned}$$

Here δ_{s+1} and σ_{s+1} define iterated odd respectively even linear combinations at the $(s+1)$-th height level of H_m,

$$\begin{aligned} \delta_{s+1}(2i-1) &= \sigma_s(2i-1)-\sigma_s(2^{m-s}-(2i-1)), & (18)\\ \sigma_{s+1}(2i-1) &= \sigma_s(2i-1)+\sigma_s(2^{m-s}-(2i-1)), & (19)\\ & \quad s=0,1,\cdots,m-2, \quad i=1,2,\cdots,2^{m-(s+2)} \end{aligned}$$

with the initial conditions

$$\sigma_0(2i-1)=\phi(y_{2^m,\,2i-1}), \quad i=1,2,\cdots,2^{m-1}, \tag{20}$$

which are defined by the newly added integrand values under polynomial degree doubling.

The *initial conditions* which complete the recurrence relations (13)–(15) are defined at the reduced abscissas, $y_{2,1}=1$, $y_{2,0}=0$, $y_{2,-1}=-1$:

$$\begin{aligned} B_{2,0} &= \tfrac{1}{2}[\phi(1)+\phi(-1)]+\phi(0), & (21)\\ B_{2,2} &= \tfrac{1}{2}[\phi(1)+\phi(-1)]-\phi(0), & (22)\\ B_{2,1} &= \tfrac{1}{2}[\phi(1)-\phi(-1)]. & (23) \end{aligned}$$

The equation (16) represents the p-th component $(p=1,2,\cdots,2^{m-(s+2)})$ of the vector

$$C_{s+1}^{(m)}=(C_{2^m,2^s\cdot 1},C_{2^m,2^s\cdot 3},\cdots,C_{2^m,2^s\cdot(2^{m-(s+1)}-1)})^\top . \tag{24}$$

which collects together the set of corrections generated at the $(s+1)$-th height level of H_m. If we denote

$$\Delta_{s+1}^{(m)}=(\delta_{s+1}(1),\delta_{s+1}(3),\cdots\delta_{s+1}(2^{m-(s+1)}-1))^\top . \tag{25}$$

and

$$\Theta_{s+1}^{(m)}=(T_{2p-1,2i-1})|_{p,i=1,2,\cdots.2^{m-(s+2)}}\,, \tag{26}$$

then the set of corrections (16) can be written in matrix form

$$C_{s+1}^{(m)} = \Theta_{s+1}^{(m)} \cdot \Delta_{s+1}^{(m)} . \quad s = 0, 1, \cdots, m-2, \quad m \geq 2 . \tag{27}$$

In conclusion, the straightforward computation of the coefficients (5) from the matrix product (6) which needs $2^m \times 2^m = 4^m$ multiplications, has been replaced by the computation of $m-1$ matrix products (27) which require a number of $(4^{m-1}-1)/3$ multiplications. Thus, the implementation of variable degree `CC` quadrature of degree $n \leq 32$ can be very efficient.

4 Symmetry properties inside blocks

Each operation of polynomial degree doubling in the `CC` quadrature adds a *unique* $2^{m-2} \times 2^{m-2}$ supplementary irreducible matrix $\Theta_1^{(m)}$ to the set of the existing ones within the `FCT` algorithm. These matrices can therefore be re-labeled in terms of the depth level l inside H_m as

$$\{\Theta_1^{(l+2)} | l = 0, 1, \cdots, m-2\} . \tag{28}$$

A particular element $\tau_{pj}^{(l)} \in \Theta_1^{(l+2)}$ takes the value

$$\tau_{pj}^{(l)} = T_{2p-1}(y_{2^{l+2}, 2j-1}) = y_{2^{l+2}, (2p-1)(2j-1)} = \cos[(2p-1)(2j-1)\pi/2^{l+2}]. \tag{29}$$

In view of the periodicity of the cosine function, it results that the values of the elements of $\Theta_1^{(l+2)}$ run over the set of values of the irreducible abscissas

$$\{y_{2^{l+2}, 2j-1} | j = 1, 2, \cdots, 2^{l+1}\} , \tag{30}$$

added under polynomial degree doubling from 2^{l+1} to 2^{l+2}.

The matrix $\Theta_1^{(2)}$ obtained at $l = 0$ consists of a single element, the root $y_{4,1}$ of H_m. In general, however, the operation of reduction of an arbitrary value $\tau_{pj}^{(l)}$, Eq. (29), to a value from the set (30) is time consuming. In what follows, we describe a solution of the reduction problem which makes use of the *symmetry properties* of the matrix $\Theta_1^{(l+2)}$. Besides the notation (29) of a generic element of $\Theta_1^{(l+2)}$, we will consider its genetically related sibling

$$t_{pj}^{(l)} = y_{2^{l+2}, 2^{l+1}-(2p-1)(2j-1)} = \sin[(2p-1)(2j-1)\pi/2^{l+2}]. \tag{31}$$

The *star of symmetry* of $\tau_{pj}^{(l)}$ will be defined to be the set of elements of $\Theta_1^{(l+2)}$ which equal either $\pm\tau_{pj}^{(l)}$ or $\pm t_{pj}^{(l)}$. The labels of the elements involved in such symmetry properties will be denoted as follows:

$$
\begin{array}{lll}
k = 2^l - j + 1, & l \geq 1, & j = 1, 2, \cdots, 2^{l-1}\,, \\
q = 2^l - p + 1, & l \geq 1 & p = 1, 2, \cdots, 2^{l-1}\,, \\
r = 2^{l-1} - p + 1, & l \geq 2, & p = 1, 2, \cdots, 2^{l-2}\,, \\
h = 2^{l-1} - j + 1, & l \geq 2, & j = 1, 2, \cdots, 2^{l-2}\,, \\
s = 2^l - r + 1 = 2^{l-1} + p, & l \geq 2, & p = 1, 2, \cdots, 2^{l-2}\,, \\
i = 2^l - h + 1 = 2^{l-1} + j, & l \geq 2, & j = 1, 2, \cdots, 2^{l-2}\,.
\end{array}
$$

The typical symmetry properties involved in the derivation of the symmetry star of $\tau_{jp}^{(l)}$ are summarized below:

- *Symmetry with respect to the first diagonal:*

$$\tau_{pj}^{(l)} = \tau_{jp}^{(l)}\,. \tag{32}$$

- *Symmetry with respect to the second diagonal:*

$$\tau_{kq}^{(l)} = (-1)^{p+j-1}\tau_{pj}^{(l)}\,. \tag{33}$$

- *Occurrence of a horizontal symmetry line:*

$$\tau_{jq}^{(l)} = \tau_{qj}^{(l)} = (-1)^{j-1}t_{pj}^{(l)}\,. \tag{34}$$

- *Occurrence of a vertical symmetry line:*

$$\tau_{kp}^{(l)} = \tau_{pk}^{(l)} = (-1)^{p-1}t_{pj}^{(l)}\,. \tag{35}$$

- *Symmetry with respect to second diagonal of first and third quadrant:*

$$\tau_{hr}^{(l)} = \tau_{rh}^{(l)} = \begin{cases} (-1)^{\chi+\delta_{l,2}-1}t_{pj}^{(l)} & \text{iff } p+j = 2\chi \\ (-1)^{\chi+\delta_{l,2}}\tau_{pj}^{(l)} & \text{iff } p+j = 2\chi+1 \end{cases} \tag{36}$$

$$\tau_{is}^{(l)} = \tau_{si}^{(l)} = \begin{cases} (-1)^{\chi+\delta_{l,2}}t_{pj}^{(l)} & \text{iff } p+j = 2\chi \\ (-1)^{\chi+\delta_{l,2}}\tau_{pj}^{(l)} & \text{iff } p+j = 2\chi+1 \end{cases} \tag{37}$$

- *Symmetry with respect to first diagonal of second and fourth quadrant:*

$$\tau_{ir}^{(l)} = \tau_{ri}^{(l)} = \begin{cases} (-1)^{\lambda-\delta_{l,2}}\tau_{pj}^{(l)} & \text{iff } p-j = 2\lambda \\ (-1)^{\lambda-\delta_{l,2}}t_{pj}^{(l)} & \text{iff } p-j = 2\lambda-1 \end{cases} \tag{38}$$

$$\tau_{ls}^{(l)} = \tau_{sl}^{(l)} = \begin{cases} (-1)^{\lambda+\delta_{l,2}}\tau_{pj}^{(l)} & \text{iff } p-j = 2\lambda \\ (-1)^{\lambda+\delta_{l,2}-1}t_{pj}^{(l)} & \text{iff } p-j = 2\lambda-1 \end{cases} \tag{39}$$

- *Symmetries involving diagonal elements:*

$$\tau_{pq}^{(l)} = \tau_{qp}^{(l)} = (-1)^{p-1} t_{pp}^{(l)} , \tag{40}$$
$$\tau_{rr}^{(l)} = (-1)^{p+\delta_{l,2}-1} t_{pp}^{(l)} , \tag{41}$$
$$\tau_{rs}^{(l)} = \tau_{sr}^{(l)} = (-1)^{\delta_{l,2}} \tau_{pp}^{(l)} , \tag{42}$$
$$\tau_{ss}^{(l)} = (-1)^{p+\delta_{l,2}} t_{pp}^{(l)} , \tag{43}$$
$$\tau_{qq}^{(l)} = -\tau_{pp}^{(l)} . \tag{44}$$

5 Concluding remarks

The following three main results have been established:

(i) The set of irreducible positive abscissas $\{y_{2^m,l} \mid l = 1, 2, \cdots, 2^{m-1} - 1\}$ can be ordered in a binary tree with heap ordering key. This allows their computation to machine accuracy using relationships for siblings characterized by complementary arguments.

(ii) The values of any line or column of coefficients of the matrix T in (6) run over the fundamental set (3). The heap ordering allows the splitting of T into $2^l \times 2^l$ irreducible blocks, where l denotes the depth level of the children inside the heap. This property allows the exploitation of the FFT great factorization theorem, resulting in a number of multiplications needed to compute (6) similar to the FFT result.

(iii) The internal structure of the irreducible $2^l \times 2^l$ blocks shows discrete symmetry properties which allow the definition of symmetry stars of the elements belonging to specific irreducible domains inside each block. The use of the occurring symmetry stars leads to the straightforward identification of the matrix elements thus keeping to a minimum the necessary computing effort.

The developed computer program will be discussed elsewhere.

Acknowledgments. The authors acknowledge partial support by grant 33515/2002 financed by the Romanian Ministry of Education and Research.

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