Fast Construction of the Fejer and Clenshaw-Curtis Quadrature Rules, Revisited

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Overview

1. Fejér and Chebyshev Points

Interpolatory quadrature rules over the interval $[-1,1]$:

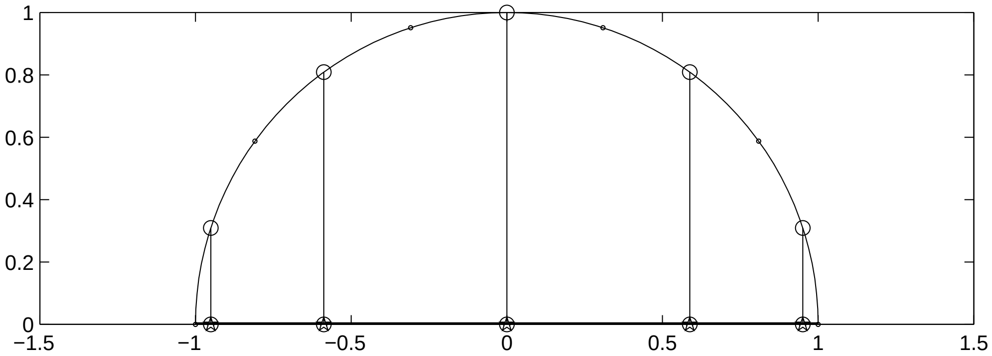
Choose N distinct nodes $x_0, x_1, \ldots, x_{N-1} \in [-1,1]$
Find N weights $w_0, w_1, \ldots, w_{N-1}$ such that

$$\int_{-1}^{1} x^l dx = \sum_{k=0}^{N-1} w_k\, x_k^l\,, \quad l = 0, 1, \ldots, N-1\,. \tag{1}$$

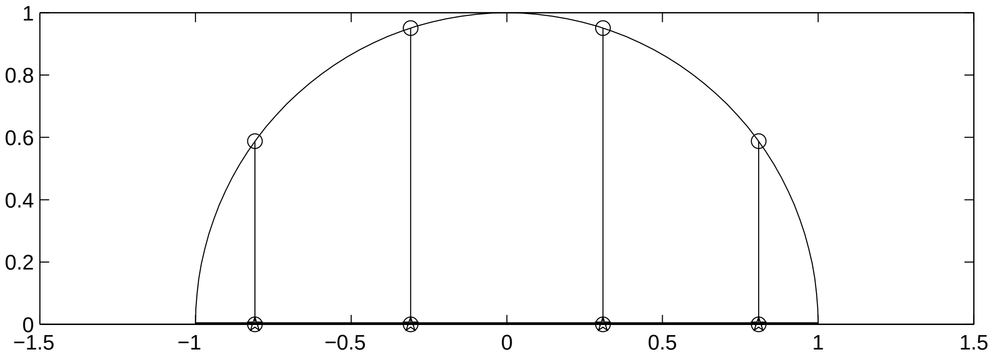
We consider the following three particular sets of nodes with $n > 1$:

1)	n	Chebyshev points (Fejér-1)	$x_k = \cos((k+\frac{1}{2})\,\frac{\pi}{n})$,	$k = 0, \ldots, n-1$
2)	$n-1$	Filippi points (Fejér-2)	$x_k = \cos(k\,\frac{\pi}{n})$,	$k = 1, \ldots, n-1$
3)	$n+1$	Clenshaw-Curtis points	$x_k = \cos(k\,\frac{\pi}{n})$,	$k = 0, .., n$

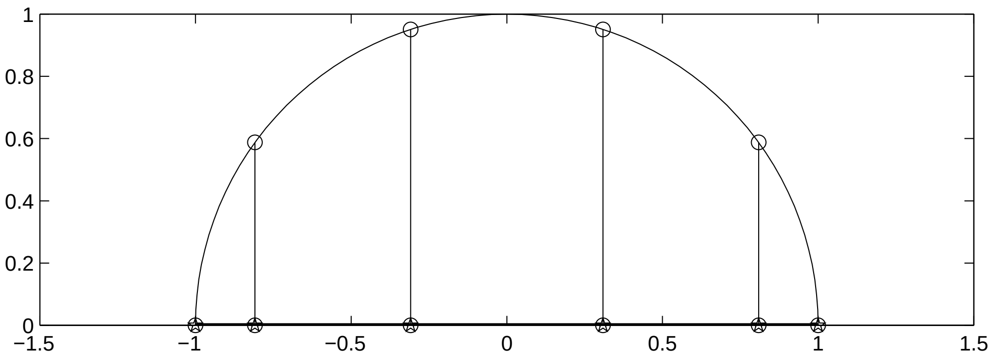
The points of the three rules with n=5



Fejer‘s first rule, n Chebyshev points



Fejer‘s second rule, n−1 Filippi points



The Clenshaw−Curtis rule, n+1 CC points

2. Earlier Results

Explicit weights: Fejér-1 or Chebyshev [1, 2, 3]:

$$w_k^{f1} = \frac{2}{n} \left(1 - 2 \sum_{j=1}^{[n/2]} \frac{1}{4j^2 - 1} \cos(j\vartheta_{2k+1}) \right) , \quad k = 0, 1, \dots, n-1 ,$$

Fejér-2 or Filippi [1, 2]:

$$w_k^{f2} = \frac{4}{n} \sin\vartheta_k \sum_{j=1}^{[n/2]} \frac{\sin\left((2j-1)\vartheta_k\right)}{2j-1} , \quad \vartheta_k = k\,\frac{\pi}{n} , \quad k = 0, 1, \dots, n ,$$

Clenshaw-Curtis [1]:

$$w_k^{cc} = \frac{q_k}{n} \left(1 - \sum_{j=1}^{[n/2]} \frac{p_j}{4j^2 - 1} \cos(2j\vartheta_k) \right) , \quad k = 0, 1, \dots, n ,$$

where the coefficients p_j, q_k are defined as (q_k erroneous in Ref. [1])

$$p_j = \begin{cases} 1, & j = n/2 \\ 2, & j < n/2 \end{cases} , \quad q_k = \begin{cases} 1, & k = 0 \mod n \\ 2, & \text{otherwise} . \end{cases}$$

A few references

1. P. J. Davis and P. Rabinowitz, 1984: *Methods of Numerical Integration*. Academic Press, San Diego, Second Edition, 612 pp. In particular: p. 84 - 86.
2. L. Fejér, 1933: *Mechanische Quadraturen mit positiven Cotesschen Zahlen*. Math. Z. **37**, 287-309.
3. W. Gautschi, 1967: *Numerical quadrature in the presence of a singularity*. SIAM J. Numer. Anal. **4**, 357-362.
4. L. N. Trefethen, 2008: *Is Gauss quadrature better than Clenshaw-Curtis?* SIAM Review **50**, 67-87.
5. J. Waldvogel, 2006: *Fast construction of the Fejer and Clenshaw-Curtis quadrature rules*. BIT Num. Math. **46**, 195-202.

Comments on Reference 5 and this note

Abstract, Ref. [5]. We present an elegant algorithm for stably and quickly generating the weights of Fejér's quadrature rules and of the Clenshaw-Curtis rule. The weights for an arbitrary number of nodes are obtained as the discrete Fourier transform of an explicitly defined vector of rational or algebraic numbers. Since these rules have the capability of forming nested families, some of them have gained renewed interest in connection with quadrature over multi-dimensional regions (see, e.g., Ref. [4]).

In this revisiting note we present new derivations of the FFT algorithms for the weights presented in Ref. [5]. These derivations are no longer based on the classical closed forms of p. 5, but go back to the original problem of p. 3, only using orthogonal polynomials, martix algebra, and discrete Fourier transforms as tools. The algorithm of Ref. [5] for the CC weights is simplified.

3. Orthogonal Polynomials

Assume the nodes $x_0, x_1, \ldots, x_{n-1}$ are the zeros of a member of a family of orthogonal polynomials. As a model we use the Chebyshev polynomials $T_l(x)$ defined by

$$T_l\big(\cos(\varphi)\big) = \cos(l\,\varphi)\,, \quad l = 0, 1, \ldots \ ;$$

then the zeros of $T_l(x)$ are

$$x_k = \cos\Big((k + \frac{1}{2})\,\frac{\pi}{l}\Big)\,, \quad k = 0, 1, \ldots, l-1\,,$$

i.e. exactly the Chebyshev or Fejér-1 points of order l.

Goal: Find the weights w_k in the quadrature formula

$$\int_{-1}^{1} f(x)\,dx = \sum_{k=0}^{n-1} w_k\, f(x_k) + R_n\,. \tag{2}$$

Exactness condition

We assume f to be a polynomial of degree $n-1$, represented as a finite series in T_l,

$$f(x) = \sum_{l=0}^{n-1} a_l \, T_l(x) \, .$$

Then the exactness conditions (1) may be replaced by

$$b_l = \sum_{k=0}^{n-1} T_l(x_k) \, w_k \, , \quad l = 0, \ldots n-1 \, . \tag{3}$$

where b_l $(l = 0, 2, 3, \ldots)$ is given by

$$b_l := \int_{-1}^{1} T_l(x) \, dx = \frac{1 + (-1)^l}{1 - l^2} = \big(2, 0, -\frac{2}{3}, 0, -\frac{2}{15}, 0, -\frac{2}{35}, 0, \ldots\big) \, .$$

Matrix algebra

By introducing the column vectors

$$\mathbf{b} = (b_0, \ldots, b_{n-1})^T, \quad \mathbf{w} = (w_0, \ldots, w_{n-1})^T$$

and the square matrix

$$\mathbf{V} = \Big(T_l(x_k)\Big) = \cos\Big(l\ (k + \frac{1}{2})\ \frac{\pi}{n}\Big),$$

where $l = 0, \ldots, n-1,\ k = 0, \ldots, n-1$, the system (3) of linear equations reads (note that here the range of the indices is $[0, n-1]$)

$$\mathbf{V} \cdot \mathbf{w} = \mathbf{b}\,. \tag{4}$$

The matrix $\mathbf{V}$ is almost orthogonal: $\mathbf{V}$ satisfies

$$\mathbf{V} \cdot \mathbf{V}^T = n \cdot \mathbf{D}^{-1} \quad \text{with} \quad \mathbf{D} = \mathrm{diag}\big((1, 2, 2, 2, \ldots)\big)\,.$$

Proof by trigonometric identities.

4. The Fourier Transform of the Weight Vector

As a consequence of the previous equation, the matrix $\frac{1}{\sqrt{n}}\sqrt{\mathbf{D}}\,\mathbf{V}$ is orthogonal, and Equ. (4) can be solved for $\mathbf{w}$ without matrix inversion:

$$\mathbf{w} = \frac{1}{n}\,\mathbf{V}^T\,\mathbf{D}\,\mathbf{b}\,.$$

Consider now the Fourier transform

$$\mathbf{v} := \mathbf{F}(\omega)\,\cdot\,\mathbf{w} = \mathbf{M}\,\cdot\,\mathbf{b} \tag{5}$$

of the weight vector $\mathbf{w}$, where $\omega = \exp(-\frac{2\,\pi\,i}{n})$ and

$$\mathbf{F}(\omega) = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & \omega & \cdots & \omega^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{n-1} & \cdots & \omega^{(n-1)^2} \end{pmatrix} = \left(\omega^{k\,l}\right), \quad k, l = 0, \ldots, n-1\,.$$

The matrix $\mathbf{M}$ is given by

$$\mathbf{M} = \frac{1}{n}\,\mathbf{F}(\omega)\,\mathbf{V}^T\,\mathbf{D}\,. \tag{6}$$

The DFT matrix

Let $\omega = \exp(-\frac{2\,\pi\,i}{n})$, then the matrix $\mathbf{F}(\omega)$ of the discrete Fourier transform of order n is defined as

$$\mathbf{F}(\omega) = \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & \omega & \cdots & \omega^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & \omega^{n-1} & \cdots & \omega^{(n-1)^2} \end{pmatrix} = \left(\omega^{k\,l}\right), \quad k, l = 0, \ldots, n-1\,.$$

The matrix of the inverse Fourier transform is $\frac{1}{n}\,\mathbf{F}(\omega^{-1}) = \frac{1}{n}\,\mathbf{F}(\bar{\omega})$, therefore we have

$$\mathbf{F}(\omega) \cdot \mathbf{F}(\omega^{-1}) = n \cdot \mathbf{I} \quad \text{with} \quad \mathbf{I} = n \times n \text{ unit matrix}\,. \tag{7}$$

5. Fejér's First Rule or Chebyshev Points

The matrix $\mathbf{M}$ defined in Equ. (6) has a simple structure. In view of the vanishing components in $\mathbf{b}$ it suffices to consider the submatrix $\mathbf{H} = \big(h_{l,j}\big)$ of $\mathbf{M}$ consisting of the even columns of $\mathbf{M} = \big(m_{l,j}\big)$:

$$h_{l,j} = m_{l,2\,j} \quad \text{with} \quad 0 \le j \le \frac{n-1}{2}\,.$$

Let $\alpha = \dfrac{2\,\pi}{n}$, $\omega = \exp(-i\,\alpha)$; for simplicity we use $n = 4$. Then

$$\mathbf{V}^T\,\mathbf{D} = \begin{pmatrix} 1 & 2\cos(\frac{1}{4}\alpha) & 2\cos(\frac{1}{2}\alpha) & 2\cos(\frac{3}{4}\alpha) \\ 1 & 2\cos(\frac{3}{4}\alpha) & 2\cos(\frac{3}{2}\alpha) & 2\cos(\frac{9}{4}\alpha) \\ 1 & 2\cos(\frac{5}{4}\alpha) & 2\cos(\frac{5}{2}\alpha) & 2\cos(\frac{15}{4}\alpha) \\ 1 & 2\cos(\frac{7}{4}\alpha) & 2\cos(\frac{7}{2}\alpha) & 2\cos(\frac{21}{4}\alpha) \end{pmatrix}. \qquad (8)$$

Now, use $2 \cdot \cos(t\,\alpha) = \omega^{-t} + \omega^{t}$ and the Fourier identity (7):

Fejér-1 or Chebyshev weights

In the case $n = 4$ we obtain

$$\mathbf{H} = \frac{1}{n}\,\mathbf{F}(\omega)\,\bigl(\mathbf{V}^T\,\mathbf{D}\bigr)_{\mathrm{even}} = \Bigl(\mathbf{e}_0\,,\ \omega^{-1/2}\,\mathbf{e}_1 + \omega^{1/2}\,\mathbf{e}_3\Bigr)\,,$$

where $\mathbf{e}_j$ is the jth basis vector, $\bigl(\mathbf{e}_j\bigr)_l = \delta_{jl}\,,\ 0 \le j, l \le n-1\,.$

For n Chebyshev points, Equ. (5) now leads to an explicit expression for the lth component ${v^{f1}}_l$ of the vector $\mathbf{v} = \mathbf{v}^{f1}$:

$$\boxed{{v^{f1}}_l = \frac{2\ s_l}{1 - 4\,m_l^2}\ \ \exp(i\,l\,\frac{\pi}{n})\,, \quad l = 0, 1, \ldots, n-1}\,, \tag{9}$$

where $\quad m_l = \min(l, n-l)\,, \quad s_l = \mathrm{sign}(\frac{n}{2} - l)\,.$

The Fejér-1 weights are obtained by inverse Fourier transform:

$$\mathbf{w}^{f1} = \frac{1}{n}\,\mathbf{F}(\omega^{-1}) \cdot \mathbf{v}^{f1}\,.$$

6. Fejér's second rule or Filippi points

In the case of the Fejér-2 (Filippi) and Clenshaw-Curtis nodes we use expansions with respect to Chebyshev polynomials of the second kind,

$$U_l\big(\cos(\varphi)\big) = \frac{\sin(l\,\varphi)}{\sin(\varphi)}\,, \quad l = 1, 2, \ldots\,,$$

since $x_k = \cos(\frac{k\,\pi}{l})$ are zeros of $U_l(x)$. First, consider the case $k = 1, 2, \ldots, n-1$ of $l = n-1$ nodes x_k. For defining the weights w_k in Equ. (2) we now expand the integrand $f(x)$ as

$$f(x) = \sum_{l=1}^{n-1} a_l\; U_l(x)\,.$$

The exactness conditions (3) then become

$$b_l = \sum_{k=1}^{n-1} U_l(x_k)\, w_k\,, \quad l = 1, 2, \ldots, n-1\,, \tag{10}$$

Fejér 2, matrix algebra 1

with

$$b_l := \int_{-1}^{1} U_l(x)\,dx = \frac{1-(-1)^l}{l} = \left(2, 0, \frac{2}{3}, 0, \frac{2}{5}, 0, \frac{2}{7}, 0, \ldots\right).$$

The matrix $\mathbf{V}$ in (4), $\mathbf{V} \cdot \mathbf{w} \ = \ \mathbf{b}$, now becomes (indices ≥ 1, as usual)

$$\mathbf{V} = \Big(U_l(x_k)\Big) = \left(\frac{\sin\left(l\ k\ \frac{\pi}{n}\right)}{\sin\left(k\ \frac{\pi}{n}\right)}\right), \quad l,\, k = 1, 2, \ldots, n-1\,. \qquad (11)$$

Denoting $\mathbf{D} := \mathrm{diag}\Big(\big(\sin(\frac{\pi}{n}), \ldots, \sin((n-1)\,\frac{\pi}{n})\big)\Big)$ and denoting the matrix of the numerators by $\mathbf{V_0}$, we have

$$\mathbf{V} = \mathbf{V_0} \cdot \mathbf{D}^{-1}\,.$$

Furthermore, trigonometric identities imply that $\sqrt{\frac{2}{n}}\,\mathbf{V_0}$ is orthogonal.

Fejér 2, matrix algebra 2

Solving Equ. (4) for $\mathbf{w}$ now yields the linear transformation $\mathbf{b} \mapsto \mathbf{w}$,

$$\mathbf{w} = \frac{2}{n}\, \mathbf{D}\, \mathbf{V_0}^T\, \mathbf{b}\,. \tag{12}$$

It is essential to supplement the vector $\mathbf{w}$ of weights by a vanishing 0th component, $\mathbf{w_0}^T := \left(0, \mathbf{w}^T\right)$, in order to be able to work with Fourier transforms of order n. Then we have $\mathbf{w_0} = \frac{2}{n}\, \mathbf{D_0}\, \mathbf{V_0}^T\, \mathbf{b}$ where $\mathbf{D_0}$ is the rectangular matrix obtained by supplementing $\mathbf{D}$ by a 0th row of zeros. Now Equ. (5), $\mathbf{F}(\omega)\, \mathbf{w} = \mathbf{M}\, \mathbf{b}$, implies

$$\mathbf{M} := \frac{2}{n}\, \mathbf{F}(\omega)\, \mathbf{D_0}\, \mathbf{V_0}^T\,,$$

where M is an $n \times n$ matrix. In analogy to Equ. (8) consider $\left(2\, \mathbf{D_0}\, \mathbf{V_0}^T\right)_{\mathrm{odd}}$, written in terms of $\alpha = \frac{2\,\pi}{n}$, this time for $n = 5$:

Fejér 2, matrix algebra 3

$$2\,\mathbf{D_0}\,\mathbf{V_0}^T = \begin{pmatrix} 1-\cos(0) & 0 & \cos(0)-\cos(0) & 0 \\ 1-\cos(\alpha) & * & \cos(\alpha)-\cos(2\alpha) & * \\ 1-\cos(2\alpha) & * & \cos(2\alpha)-\cos(4\alpha) & * \\ 1-\cos(3\alpha) & * & \cos(3\alpha)-\cos(6\alpha) & * \\ 1-\cos(4\alpha) & * & \cos(4\alpha)-\cos(8\alpha) & * \end{pmatrix}. \qquad (13)$$

Now, again use $2\cdot\cos(t\,\alpha) = \omega^{-t} + \omega^t$ with $\omega = \exp(-i\,\alpha)$ and the Fourier identity (7). In the case $n = 5$ we obtain

$$\mathbf{H} = \frac{2}{n}\,\mathbf{F}(\omega)\left(\mathbf{D_0}\,\mathbf{V_0}^T\right)_{\mathrm{odd}} = \left(\mathbf{e}_1 - \frac{\mathbf{e}_2+\mathbf{e}_5}{2}\,,\ \frac{\mathbf{e}_2-\mathbf{e}_3-\mathbf{e}_4+\mathbf{e}_5}{2}\right),$$

where $\mathbf{e}_j$ again is the jth basis vector, $\left(\mathbf{e}_j\right)_l = \delta_{jl}$.

Fejér-2 or Filippi weights

For $n-1$ Filippi points, this procedure leads to the explicit expression

$$\boxed{{v^{f2}}_l = \frac{2\,\sigma_l}{1-4\,m_l^2}\,, \quad l=0,1,\ldots,n-1} \tag{14}$$

for the lth component ${v^{f2}}_l$ of the vector $\mathbf{v}=\mathbf{v}^{f2}$, where

$$\begin{aligned} m_l &= \min(l, n-l) \\ \sigma_l &= 1 + f_l \cdot \big(n - (\tfrac{n}{2}+1)\operatorname{mod}(n,2)\big) \\ f_l &= |\, l - \tfrac{n}{2}\,| < 1 \quad \text{(=1 if inequality is true, =0 otherwise)}\,. \end{aligned}$$

The Fejér-2 weights are again obtained by inverse Fourier transform:

$$\mathbf{w}^{f2} = \frac{1}{n}\,\mathbf{F}(\omega^{-1}) \cdot \mathbf{v}^{f2}\,.$$

7. The Clenshaw-Curtis rule

is closely related to the Fejér-2 (Filippi) rule; it merely contains the boundary points $x = \pm 1$ in addition, totally $n+1$ nodes.

Denoting the weights by $u_k\,,\ k = 0, 1, \ldots, n$, the exactness conditions (10) now become

$$b_l = \sum_{k=0}^{n} U_l(x_k)\, u_k\,, \quad l = 1, 2, \ldots, n+1\,,$$

where the matrix $\mathbf{V} = \big(v_{lk}\big) = \big(U_l(x_k)\big)$ is defined in Equ. (11).

For simplicity we use the the odd case $n = 3$ and the even case $n = 4$ as models and show the last three exactness conditions, using the relations $U_l(1) = l,\ U_l(-1) = l\,(-1)^{l-1}$:

CC rule, matrix algebra 1 n=3 n=4

$$\begin{array}{ll}
2\,u_0 \;+v_{21}\,u_1+v_{22}\,u_2 -2\,u_3 = 0 & 3\,u_0 \;+v_{31}\,u_1+v_{32}\,u_2+v_{33}\,u_3+3\,u_4=\frac{2}{3} \\
3\,u_0 \qquad\qquad\qquad\qquad +3\,u_3 = \frac{2}{3} & 4\,u_0 \qquad\qquad\qquad\qquad\qquad -4\,u_4 = 0 \\
4\,u_0 \;-v_{21}\,u_1-v_{22}\,u_2 -4\,u_3 = 0 & 5\,u_0 \;-v_{31}\,u_1-v_{32}\,u_2-v_{33}\,u_3+5\,u_4=\frac{2}{5}
\end{array}$$

$$\Longrightarrow \qquad u_0 = u_3 = \tfrac{1}{3\cdot 3} \qquad\qquad u_0 = u_4 = \tfrac{1}{3\cdot 5}$$

$$\text{In summary :} \qquad \boxed{u_0 = u_n = \frac{1}{n^2-1+\mathrm{mod}(n,2)}}\,. \tag{15}$$

The remaining CC weights $\mathbf{u} = \big(u_1, \ldots, u_{n-1}\big)^T$ satisfy the equation

$$\mathbf{V}\cdot\mathbf{u} = \mathbf{b} - u_0\,\mathbf{c} \quad \text{with} \quad \mathbf{c} = 2\cdot\big(1,0,3,0,5,0,7,0,\ldots\big)^T. \tag{16}$$

Clenshaw-Curtis weights

Applying the linear transformation (12) to $\mathbf{c}$ instead of $\mathbf{b}$ yields the vector

$$\mathbf{v} = \sum_{l=0}^{n-1} \tau_l \; \mathbf{e}_l$$

where

$$\tau_l = 1 - f_l \cdot n \left(2 - \mathrm{mod}(n,2)\right) \quad \text{with} \quad f_l = \left| l - \frac{n}{2} \right| < 1\,,$$

f_l as in Equ. (14). By using Equ. (16), the procedure of Section 6 finally yields the Clenshaw-Curtis weights as the inverse Fourier transform of the vector $\mathbf{v}^{CC}$ with components

$$\boxed{ {v^{CC}}_l = \frac{2}{1 - 4\,m_l^2} - u_0\,, \quad l = 0, 1, \ldots, n-1 }\;. \tag{17}$$

MATLAB code

```
function [wcc,wf1,wf2] = fejer1(n)
% Weights of the Clenshaw-Curtis, Fejer1, and Fejer2 quadratures by DFTs
% n>1. Nodes: x_k = cos(k*pi/n)
n2=mod(n,2); u0=1/(n^2-1+n2);                     % Boundary weights of CC
% Clenshaw-Curtis nodes: k=0,1,...,n;  vector of weights wcc, wcc_0=wcc_n=u0
L =[0:n-1]'; m =min(L,n-L); r=2./(1-4*m.^2);  % auxiliary vectors for all rules
vc=r-u0; wcc=ifft(vc);                              % Clenshaw-Curtis weights
%
% Chebyshev or Fejer-1 nodes: k=1/2,3/2,...,n-1/2; vector of weights wf1
s1=sign(n/2-L);                                     % auxiliary vector
v1=s1.*r.*exp(i*pi/n*L); wf1=real(ifft(v1));  % Chebyshev or Fejer-1 weights
%
% Filippi or Fejer-2 nodes: k=0,1,...,n; vector of weights wf2, wf2_0=wf2_n=0
flag=abs(n/2-L)<1; s2=1+flag*(n-(n/2+1)*n2);  % auxiliary vectors
v2=s2.*r; wf2=ifft(v2);                             % Filippi or Fejer-2 weights
```

Timings for $n = 16, 512, 521: \;\; 35, 113, 210\ \mu s \quad (63, 131, 230\ \mu s$ in Ref. 5)

8. Conclusions

- The three quadraure rules Fejér 1 (Chebyshev), Fejér 2 (Filippi), and Clenshaw-Curtis, based on nodes given by cosines of equally spaced angles, are powerful and easy-to-generate tools of numerical quadrature.
- A new theory, based on orthogonal polynomials and matrix algebra, for finding closed forms of the Fourier transforms of the weight vectors has been presented.
- On this basis the weight vectors of these quadrature rules can be efficiently generated in $O\big(n \log(n)\big)$ operations.
- The algorithms simply are the inverse Fourier transforms of the explicitly defined vectors (9), (14), and (17).