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Recurrence Relations For Computing With Modified Divided Differences

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Preface

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Abstract

Modified divided differences (MDD) provide a good way of representing a polynomial passing through points with unequally spaced abcissas. This report gives recurrence relations for computing coefficients in either the monomial or Chebyshev basis from the MDD coefficients, and for computing the MDD coefficients for either the differentiated or the integrated polynomial. The latter operation is likely to be useful if MDD are used in a method for solving stiff differential equations.

CONTENTS

1. Introduction

A modification of divided differences was first suggested by Blanch [1] as a means of getting some of the desirable characteristics of differences when working with unequal intervals. Modified divided differences of the form used here were introduced in [2] and developed further in [3]. Shampine and Gordon use them in [4] and Jackson [5] has made a careful study of related computational approaches, concluding that the form used here is best. Jackson has also showed that the round-off characteristics of these modified divided differences are excellent.

The polynomial of lowest degree passing through the points $(t_i, w(t_i))$, $i = n, n-1, \ldots, n-q+1$ can be expressed in terms of the MDD coefficients $\phi_i(n)$ according to the formula

$$(1) \qquad P_{q-1,n}(t) = P_{q-1,n}(t_n + h_h\tau) = \sum_{i=0}^{q-1} \phi_i(n)\, c_{i,n}(\tau)$$

Where we use notation similar to that in [3].

(2)
$$
\begin{aligned}
h_i &= t_i - t_{i-1} \\
\tau &= (t-t_n)/h_n \\
\xi_i(n) &= h_n + h_{n-1} + \ldots + h_{n-i} = t_n - t_{n-i-1} = \xi_{i-1}(n-1) + h_n \\
\alpha_i(n) &= h_n/\xi_i(n) \\
\beta_0(n) &= 1 \\
\beta_{i+1}(n) &= (\xi_i(n)/\xi_i(n-1))\beta_i(n) \\
\phi_0(n) &= w(t_n) \\
\phi_{i+1}(n) &= \phi_i(n) - \beta_i(n)\phi_i(n-1) \\
c_{0,n} &= 1 \\
c_{1,n} &= \alpha_0(n)\tau = \tau \\
c_{i,n} &= [\alpha_{i-1}(n)\tau + \xi_{i-2}(n)/\xi_{i-1}(n)]\ c_{i-1,n}, \quad i \geq 2
\end{aligned}
$$

Here we think of the $\phi_i(n)$ as coefficients of a polynomial expressed in terms of the basis polynomials $c_{i,n}(\tau)$. In [3], the orientation was focused more on the $\phi_i(n)$ which are the modified divided differences of w computed at $t=t_n$.

2. Converting to Coefficients for Other Basis Polynomials

Salzer [6] gives a general recurrence for converting coefficients for one set of polynomial basis functions to coefficients for another set of polynomial basis functions. In Salzer's notation the $c_i(\tau)$ (Henceforth we no longer explicitly include n when referring to the various parameters defined in eq. (2)) satisfy the recurrence.

(3)
$$c_{m+1}(\tau) + (a(m) + b(m)\tau)\ c_m(\tau) + c(m)\ c_{m-1}(\tau) = 0$$

where
$$
\begin{aligned}
a(0) &= 0,\ a(m) = \xi_{m-1}/\xi_m,\ m \geq 1 \\
b(m) &= -\alpha_m \\
c(m) &= 0
\end{aligned}
$$

and for the monomial basis, $Q_m(\tau) = \tau^m$, $A(m) = C(m) = 0$, $B(m) = -1$. Simply substituting in his eq. (22) yields (his $n = q-1$)

(4)
$$a_0^{(0)} = \phi_{q-1}$$

$$a_0^{(k+1)} = \phi_{q-k-2} + (\xi_{q-k-3}/\xi_{q-k-2})\, a_0^{(k)}$$

$$a_m^{(k+1)} = \alpha_{q-k-2} a_{m-1}^{(k)} + (\xi_{q-k-3}/\xi_{q-k-2})\, a_m^{(k)}, \quad m = 1, 2, \ldots, k$$

$$a_{k+1}^{(k+1)} = \alpha_{q-k-2}\, a_k^{(k)}$$

where $k = 0, 1, \ldots, q-2$, and $\xi_{-1} = 0$. The desired coefficients are then $a_m^{(q-1)}$, $m=0,1,\ldots, q-1$. Since $\alpha_0 = 1$, $a_m^{(q-1)} = a_{m-1}^{(q-2)}$ for $m > 0$. Substituting $(\hat{a}_{m+1}^{(k)}/\alpha_{q-k-2})$ for $a_m^{(k)}$, (4) simplifies to

(5)
$$\hat{a}_1^{(0)} = \alpha_{q-2}\phi_{q-1}$$

$$\hat{a}_1^{(k+1)} = \alpha_{q-k-3}\phi_{q-k-2} + \hat{a}_1^{(k)}$$

$$\hat{a}_{m+1}^{(k+1)} = \alpha_{q-k-3}\hat{a}_m^{(k)} + \hat{a}_{m+1}^{(k)}, \quad m=1, 2, \ldots, k$$

$$\hat{a}_{k+2}^{(k+1)} = \alpha_{q-k-3}\, \hat{a}_{k+1}^{(k)}$$

where $k=0, 1, \ldots, q-3$. The desired coefficients are then given by ϕ_0, $\hat{a}_m^{(q-2)}$, $m=1, 2, \ldots, q-1$. The operations in (5) require only a single vector of storage since ϕ_m and $\hat{a}_{q+m-k-2}^{(k)}$, $k=0, 1, \ldots$ can all occupy the same location. Denoting this location by ψ_m, we have

(6)
$$\psi_{q-1} = \alpha_{q-2}\psi_{q-1}$$

$$\left.\begin{aligned} &\psi_{q+m-k-2} = \alpha_{q-k-3}\psi_{q+m-k-2} + \psi_{q+m-k-1}, \quad m=0,1, \ldots, k \\ &\psi_{q-1} = \alpha_{q-k-3}\psi_{q-1} \end{aligned}\right\} \quad k=0, 1, \ldots, q-3$$

One gets a similar recurrence from eq. (5.11) of [3] by replacing the iteration indices k=1, 2, ..., i; i=q-1, ..., 1 with i=q-1, ..., k; k=1, 2, ..., q-1, then replacing i with q+k-j-1 and then interchanging the order of iteration indices once again.

For the case of converting to the Chebyshev basis, we have A(m) = 0, B(0) = -1, B(m) = -2, m > 0, C(m) = 1. Substituting as before, and then setting $(\hat{a}_0^{(k)}/2\alpha_{q-k-2}) = a_0^{(k)}$, $(\hat{a}_m^{(k)}/\alpha_{q-k-2}) = a_m^{(k)}$, m > 0, one obtains

$$
\begin{aligned}
(7)\qquad \hat{a}_0^{(0)} &= 2\alpha_{q-2}\phi_{q-1} \\
\hat{a}_0^{(k+1)} &= \alpha_{q-k-3}\,[2\phi_{q-k-2} + \hat{a}_1^{(k)}] + \hat{a}_0^{(k)} = (2\alpha_{q-3}\phi_{q-2} + \hat{a}_0^{(0)} \text{ if } k=0) \\
\hat{a}_m^{(k+1)} &= (1/2)\alpha_{q-k-3}\,[\hat{a}_{m-1}^{(k)} + \hat{a}_{m+1}^{(k)}] + \hat{a}_m^{(k)}, \quad m=1, 2, \ldots, k-1 \\
\hat{a}_k^{(k+1)} &= (1/2)\alpha_{q-k-3}\,\hat{a}_{k-1}^{(k)} + \hat{a}_k^{(k)} \\
\hat{a}_{k+1}^{(k+1)} &= (1/2)\alpha_{q-k-3}\,\hat{a}_k^{(k)}
\end{aligned}
$$

where k=0, 1, ..., q-3, and the desired coefficients are $\hat{a}_m^{(q-1)}$ given by

$$
\begin{aligned}
(8)\qquad \hat{a}_0^{(q-1)} &= \phi_0 + (1/2)\,\hat{a}_1^{(q-2)} \\
\hat{a}_m^{(q-1)} &= (1/2)\,[\hat{a}_{m-1}^{(q-2)} + \hat{a}_{m+1}^{(q-2)}], \quad m=1, 2, \ldots, q-3 \\
\hat{a}_{q-2}^{(q-1)} &= (1/2)\,\hat{a}_{q-3}^{(q-2)} \\
\hat{a}_{q-1}^{(q-1)} &= (1/2)\,\hat{a}_{q-2}^{(q-2)}
\end{aligned}
$$

As before, the calculations in (7) can be done in a single vector of storage as follows (initially $\psi_m = \phi_m$)

(9) $$\psi_{q-1} = 2\alpha_{q-2}\psi_{q-1}$$

$$\psi_{q-2} = 2\alpha_{q-3}\psi_{q-2} + \psi_{q-1}$$

$$\psi_{q-1} = (1/2)\alpha_{q-3}\psi_{q-1}$$

$$\left.\begin{array}{l} \psi_{q-k-2} = \alpha_{q-k-3}\,[2\psi_{q-k-2} + \psi_{q-k}] + \psi_{q-k-1} \\ \psi_{q-k-2+m} = (1/2)\alpha_{q-k-3}[\psi_{q-k-2+m} + \psi_{q-k+m}] + \psi_{q-k-1+m}, \\ \qquad\qquad m=1,\ 2,\ \ldots,\ k-1 \\ \psi_{q-2} = (1/2)\alpha_{q-k-3}\psi_{q-2} + \psi_{q-1} \\ \psi_{q-1} = (1/2)\alpha_{q-k-3}\psi_{q-1} \end{array}\right\} k=1,\ 2,\ \ldots,\ q-3$$

The final Chebyshev coefficients are then obtained, using (8) as follows

(10) $$\psi_0 = \psi_0 + (1/2)\psi_1$$

$$\psi_m = (1/2)[\psi_m + \psi_{m+2}],\ m=1,\ \ldots,\ q-1$$

$$\psi_{q-2} = (1/2)\psi_{q-2}$$

$$\psi_{q-1} = (1/2)\psi_{q-1}$$

If one is using the method outlined in [3] or the code in [4], the α's are available at the time of integration. Clearly some time can be saved in the above calculations if τ is redefined to be $(t-t_n)/2h$, since this has the effect of setting $b_m = -2\alpha_m$ and as a result the multiplications by 1/2 are eliminated. (For this case, simply replace α_i by $2\alpha_i$ in (9), and replace all 1/2's in (10) with 1. For $\tau = t - t_n$, divide by h everyplace we just indicated a multiplication by 2.)

If one wants to approximate the solution of a differential equation by a Chebyshev polynomial, and thus wants to get the coefficients for the integrated polynomial, one can save a little computation by computing the integrated coefficients after the calculations indicated in (7) or (9). Thus for $3 \leq n \leq q-4$ one has for $\tilde{a}_n$, the n-th coefficient of the integrated polynomial

$$\tilde{a}_n = \begin{cases} (1/2n)(\hat{a}_{n-1}^{(q-1)} - \hat{a}_{n+1}^{(q-1)}) \text{ after (8)} \\ \\ (1/4n)(\hat{a}_{n-2}^{(q-2)} - \hat{a}_{n+2}^{(q-2)}) \text{ after (7)} \end{cases} \tag{11}$$

3. <u>Computing Coefficients for the Integrated or Differentiated Polynomial</u>

When integrating stiff equations, the best integration method is different depending on how far the most active component is from its local equilibrium point. If a procedure such as that in [3] is used, changes in the method involve either getting coefficients for the integrated polynomial when leaving a transient region, or for the differentiated polynomial when a transient is encountered. We have also encountered a desire for such a transformation in another context.

The best general algorithm we have been able to find for the case of variable stepsize involves running through the recurrences in (6), replacing ψ_k with ψ_{k-1}/k, k=q, ..., 1 for integration (or with $(k+1)\psi_{k+1}$, k=0, 1, ..., q-2 for differentiation). For integration, ψ_0 is set to the constant of integration. Then simply run the recurrence (6) in reverse order

$$(12)\qquad \left.\begin{aligned} &\psi_{q'-1} = \psi_{q'-1}/\alpha_{q'-k-3} \\ &\psi_{q'+m-k-2} = (\psi_{q'+m-k-1} - \psi_{q'+m-k-2})/\alpha_{q'-k-3},\ m=k,\ \ldots,\ 0 \\ &\psi_{q'-1} = \psi_{q'-1}/\alpha_{q'-k-3} \end{aligned}\right\}\ k=q'-2,\ \ldots,\ 0$$

where $q' = q+1$, for integration, and $q'=q-1$ for differentiation. In the case of a constant stepsize, one can accomplish this goal more efficiently by repeated differencing of the corrector equation

$$(13)\qquad \nabla y_n = h \sum_{k=0}^{q-1} \gamma_k^* \nabla^k y'_n$$

Thus

$$(14)\qquad \nabla^j y_n = h \sum_{k=0}^{q-j} \gamma_k^* \nabla^{k+j-1} y'_n\ ,\ j=1,\ 2,\ \ldots,\ q,$$

and the reverse operation simply involves treating eq. (14) as a triangular system to be solved for the $\nabla^k y'_n$.

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