THE DETERMINATION OF DERIVATIVE PARAMETERS
FOR A
MONOTONIC RATIONAL QUADRATIC INTERPOLANT

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Abstract

Explicit formulae are developed for determining the derivative parameters of a monotonic interpolation method of Gregory and Delbourgo (1982).
1. Introduction

In Gregory and Delbourgo (1982) a $C^1$ monotonic interpolation method is described which interpolates given monotonic data. The purpose of this note is to develop explicit formulae for determining the derivative parameters of the scheme from the given function valued data. Let $(x_i, f_i)$, $i = 1, ..., n$, denote the data, where $x_1 < x_2 < ... < x_n$, and assume that $f_1 \leq f_2 \leq \ldots \leq f_n$ (monotonic increasing data). Then derivative parameters $d_i$, $i = 1, ..., n$, are to be determined at the knots $x_i$, $i = 1, ..., n$, which satisfy the necessary monotonicity conditions $d_i \geq 0$, $i = 1, ..., n$. The interpolation method then constructs a monotonic piecewise rational quadratic function $s(x)$ such that

$$s(x_i) = f_i \quad \text{and} \quad s^{(1)}(x_i) = d_i, \quad i = 1, ..., n.$$  \hspace{1cm} (1.1)

This function is defined, for $x \in [x_i, x_{i+1}]$, $i = 1, ..., n-1$, by

$$s(x) = \frac{\Delta_i \cdot f_{i+1} \cdot \theta^2 + (f_{i+1} \cdot d_{i+1} + f_i \cdot d_i) \theta (1 - \theta) + \Delta_i \cdot f_i \cdot (1 - \theta)^2}{\Delta_i \cdot \theta^2 + (d_{i+1} + d_i) \theta (1 - \theta) + \Delta_i \cdot (1 - \theta)^2},$$  \hspace{1cm} (1.2)

where

$$h_i = x_{i+1} - x_i, \quad \Delta_i = (f_{i+1} - f_i) / h_i, \quad \theta = (x - x_i) / h_i.$$  \hspace{1cm} (1.3)

In the case $A = 0$ we have $s(x) = f_i$, a constant on $[x_i, x_{i+1}]$.

When $f_i = f(x_i)$, $i = 1, ..., n$, where $f$ is a strictly monotonic increasing function, the interpolant has an error bound of the form

$$|f(x) - s(x)| \leq \max_i f^{(i)}(x_i) \cdot 0(h) + 0(h^4),$$  \hspace{1cm} (1.4)

where $f \in C^4[x_1, x_n]$ and $h = \max_i \{h_i\}$. The accuracy of the interpolant is thus dependent on the accuracy of the values $d_i$ considered as approximations to the true derivations $f^{(i)}(x_i)$. Hence, given only the
function valued data, we are concerned with determining explicit derivative formulae which give non—negative approximations of appropriate orders of accuracy.

The approximations developed here also provide end conditions for the $C^2$ rational quadratic spline method of Delbourgo and Gregory (1983). The spline method determines $O(h^3)$ accurate derivative parameters $d_i$, $i = 2,...,n-1$, as the solution of a non-linear system of equations, where $d_1$ and $d_n$ are given at the ends of the knot partition. If these end derivatives are not known, then $O(h^3)$ non-negative approximations to them are required in order to preserve the optimal $O(h^4)$ accuracy of the rational spline.

2. The Derivative Formulae

Let $I_i$ denote an index set of $m$ values $j \in \{1,...,n\}$, $j \neq i$, chosen in a neighbourhood of $i$ and let $p_i(x)$ be the interpolation polynomial of degree $m$ such that $p_i(x_j) = f_j$, $j \in I_i \cup \{i\}$. Then $d_i = p_i^{(1)}(x_i)$ provides a classical method of constructing $O(h)$ derivative approximations to $f^{(1)}_i$. This method will give equation (2.1) below, which can be considered as a generalized arithmetic mean of the non-negative secant slopes $\Delta_{i,j}$, where the weights $\alpha_{i,j}$ are not, in general, all positive. Considerations regarding monotonicity lead us to study also geometric and harmonic forms for the approximations. We then have the following theorem.

**Theorem 2.1.** Let $f \in C^{m+1}[x_1,x_n]$ and $f^{(1)}(x) > 0$ on $[x_1,x_n]$. Let the index set $I_i$ of $m$ values $j \neq i$ be such that $|x_i - x_j| \leq Kh$, for all $j \in I_i$, where $h = \max\{h_i\}$ and $K$ is independent of $h$. Then $f_i^{(1)} - d_i = O(h^m)$ for each of the following generalized arithmetic, geometric and harmonic means:

$$d_i \sum_{j \in I_i} a_{i,j} \Delta_i, j,$$  \hspace{1cm} (2.1)
\[ d_i = \pi_{j \in I_i} \frac{\Delta_{i,j}}{a_{i,j}}, \quad (2.2) \]

\[ d_i = \frac{1}{\sum_{j \in I_i} a_{i,j}/\Delta_{i,j}}, \quad (2.3) \]

where

\[ \Delta_{i,j} = \frac{f_j - f_i}{x_j - x_i}, \quad (2.4) \]

\[ a_{i,j} = \pi_{k \in I_i} \left( \frac{x_k - x_i}{x_k - x_j} \right)_{k \neq j} \]

A proof of this theorem is a consequence of the two lemmas given below, but we first make some remarks concerning the behaviour of the approximations (2.1) - (2.3).

The arithmetic mean (2.1) can give negative results for all but the simplest choices of the index sets \( I_i \). The geometric form (2.2) is always non-negative and it can be shown that the harmonic mean is non-negative for most of the specific index sets used in the examples of the next section. In practical applications any negative result is replaced by the value zero.

Another problem occurs if \( \Delta_{i,j} = 0 \), since monotonicity implies \( s(x) = \text{constant} \) between \( x_i \) and \( x_j \) and hence \( d_i = 0 \). Thus if \( \lim d_i \neq 0 \) as \( \Delta_{i,j} \to 0 \) in (2.1), (2.2) and (2.3) it follows that the formulae will not define continuous functionals and the interpolants will not behave in a continuous manner with respect to changes in the data in this limiting case. The arithmetic mean (2.1) exhibits this unsatisfactory behaviour but the geometric and harmonic forms (2.2) and (2.3) are satisfactory for most of the index sets considered later.

**Lemma 2.1.** Let \( I \) denote an index set of \( m \) positive integers and let \( i, j \in I \), be \( m \) distinct non-zero values. Then the linear system in the
unknowns $\alpha_j$, defined by

\[ \sum_{j \in I} \alpha_j = 1, \quad \sum_{j \in I} \varepsilon_j^k \alpha_j = 0, \quad k = 1, \ldots, m - 1, \tag{2.6} \]

has the unique solution

\[ \alpha_{i,j} = \prod_{k \neq j}^{\pi} \left( \frac{\varepsilon_k^j}{\varepsilon_k^j - \varepsilon_j^j} \right), \quad j \in I. \tag{2.7} \]

**Proof** It suffices to prove (2.7) for the index set $I = \{1, 2, \ldots, m\}$, although different sets will be considered in our application of the lemma. The system (2.6) then assumes the form

\[
\begin{bmatrix}
1 & 1 & \cdots & 1 \\
\varepsilon_1 & \varepsilon_2 & \cdots & \varepsilon_m \\
\vdots & \vdots & \ddots & \vdots \\
\varepsilon_m^{-1} & \varepsilon_m^{-2} & \cdots & \varepsilon_m^{-1}
\end{bmatrix}
\begin{bmatrix}
\alpha_1 \\
\alpha_2 \\
\vdots \\
\alpha_m
\end{bmatrix}
\begin{bmatrix}
1 \\
0 \\
\vdots \\
0
\end{bmatrix}.	ag{2.8}
\]

The coefficient matrix has the non-zero Vandermonde determinant defined by

\[ V(\varepsilon_1, \ldots, \varepsilon_m) = \prod_{p > q}^{m} (\varepsilon_p - \varepsilon_q) \]

and (2.8) has the unique solution

\[ \alpha_j = \frac{V(\varepsilon_1, \ldots, 0, \ldots, \varepsilon_m)}{V(\varepsilon_1, \ldots, \varepsilon_j, \ldots, \varepsilon_m)} = \prod_{k=1}^{m} \left( \frac{\varepsilon_k^j}{\varepsilon_k^j - \varepsilon_j^j} \right) \]

**Lemma 2.2** Let $\lambda > 0$ and $\lambda_j > 0$ be given such that

\[ \lambda_j = \lambda + \sum_{k=1}^{m-1} b_k \varepsilon_j^k + O(\varepsilon_m), \quad j \in I, \tag{2.9} \]
where $b_k$ are constants (independent of $j$), $\varepsilon = \max |\varepsilon_j|$ and the $\varepsilon_j$ satisfy the hypotheses of Lemma 2.1. Then the generalized arithmetic, geometric and harmonic means defined by

$$A = \sum_{j \in I} a_j \lambda_j, \quad G = \sum_{j \in I} \lambda_j a^j, \quad H = \frac{1}{\sum_{j \in I} a_j \lambda j}$$

are all $O(\varepsilon^m)$ approximations to $\lambda$, where the $\alpha_j$ are defined by (2.7) of Lemma 2.1.

**Proof**

(i) Substituting (2.9) in the definition of the arithmetic mean gives

$$A = \sum_{j \in I} \alpha_j [\lambda + O(\varepsilon^m)] + \sum_{k=1}^{m-1} b^k \sum_{j \in I} a_j \varepsilon^k.$$ 

Thus $A = \lambda + O(\varepsilon^m)$ for $\alpha_j$ satisfying (2.6).

(ii) Noting that $\lambda_j > 0$ and $\lambda > 0$, we take the logarithm of the geometric mean and substitute (2.9) to give

$$\log G = \sum_{j \in I} \alpha_j \log \lambda_j$$

$$= \sum_{j \in I} \alpha_j \log \lambda + \log \left(1 + \sum_{k=1}^{m-1} \lambda^k b^k \varepsilon^k + O(\varepsilon^m)\right)$$

$$= \sum_{j \in I} \alpha_j \log \lambda + \sum_{j \in I} \alpha_j \left\{ \sum_{k=1}^{m-1} c^k \varepsilon^k + O(\varepsilon^m) \right\}$$

where the $c_k$ are constants, obtained by collecting terms of a power series expansion of the second logarithmic term. Thus $\log G - \log \lambda = O(\varepsilon^m)$, for $\varepsilon_j$ satisfying (2.6) and hence $G = \lambda + O(\varepsilon^m)$.

(iii) Noting that $\lambda \neq 0$, we take the reciprocal of the harmonic mean and substitute (2.9) to give
\[ H^{-1} = \lambda^{-1} \sum_{j=1} \alpha_j \left[ 1 + \sum_{k=1}^{m-1} \lambda^{-1}_b \varepsilon_j^k + 0(\varepsilon^m) \right]^{-1} \]

\[ = \lambda^{-1} \sum_{j=1} \alpha_j \left[ 1 + \sum_{k=1}^{m-1} \gamma_k \varepsilon_j^k + 0(\varepsilon^m) \right] \]

where the \( y_k \) are constants, obtained by collecting terms of a power series expansion of the reciprocal term. Thus \( H^{-1} = \lambda^{-1} [1 + 0(\varepsilon^m)] \), for \( \alpha_j \) satisfying (2.6) and hence \( H = \lambda + O(\varepsilon^m) \).

In our application of Lemma 2.2 the weights \( a \) will not necessarily be all positive. However, for positive weights we have the standard inequality

\[ 0 < H < G < A \]

Lemma 2.2 also holds for the case \( \lambda < 0, \lambda_j < 0, j \in I \), with the geometric mean now being defined by

\[ G = -\pi \left( -\lambda \right)^{a_j} \]

However, this result is not needed here in our treatment of monotonic increasing data.

Theorem 2.1 is an immediate consequence of Lemmas 2.1 and 2.2 since Taylor expansions about \( x_i \) of the positive secant slopes \( \Delta_{i,j} \) give

\[ \Delta_{i,j} = f_i^{(1)} + \sum_{k=1}^{m-1} b_{i,k} \varepsilon_i^k + 0(\varepsilon_i^{m}) , \quad j \in I_i , \]

(2.11)

where \( b_{i,k} = f_i^{(k+1)}/(k+1)! \) and \( \varepsilon_i = x_j - x_i \). Thus (2.11) can be used as the hypothesis (2.9) of Lemma 2.2.

In the next section we give specific examples of the application of Theorem 2.1 appropriate to the piecewise rational quadratic interpolation method.
3. **Examples and Numerical Results**

3.1 **Test problems**

We have applied the rational quadratic scheme to three monotonic increasing data sets using derivative approximations defined in the next two subsections. The first set of data is that given in Table 1 and is an example used by Fritsch and Carlson (1980). The second is that used by Pruess (1979) and is given in Table 2. The third set of data consists of points spaced at $15^\circ$ arguments over a quarter circle and is distinguished by the difficulty of an infinite gradient at an end point.

<table>
<thead>
<tr>
<th>X</th>
<th>7.99</th>
<th>8.09</th>
<th>8.19</th>
<th>8.7</th>
<th>9.2</th>
<th>10</th>
<th>12</th>
<th>15</th>
<th>20</th>
</tr>
</thead>
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<td>y</td>
<td>0</td>
<td>2.7629x10^{-5}</td>
<td>4.37498x10^{-2}</td>
<td>0.169183</td>
<td>0.469428</td>
<td>0.943740</td>
<td>0.998636</td>
<td>0.999919</td>
<td>0.999994</td>
</tr>
</tbody>
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Table 1. Fritsch-Carlson data.

<table>
<thead>
<tr>
<th>X</th>
<th>22</th>
<th>22.5</th>
<th>22.6</th>
<th>22.7</th>
<th>22.8</th>
<th>22.9</th>
<th>23</th>
<th>23.1</th>
<th>23.2</th>
<th>23.3</th>
<th>23.4</th>
<th>23.5</th>
<th>24</th>
</tr>
</thead>
<tbody>
<tr>
<td>y</td>
<td>523</td>
<td>543</td>
<td>550</td>
<td>557</td>
<td>565</td>
<td>575</td>
<td>590</td>
<td>620</td>
<td>860</td>
<td>915</td>
<td>944</td>
<td>958</td>
<td>986</td>
</tr>
</tbody>
</table>

Table 2. Pruess data.

3.2 **$O(h^3)$ interpolation methods**

Let $m = 2$. Then equations (2.1) -(2.3) give $O(h^2)$ derivative approximations with the following choices of index sets:

$$I_1 = \{2,3\} \quad \text{for} \quad d_1,$$

$$I_i = \{i-1,i+1\} \quad \text{for} \quad d_i \ , \ i = 2, \ldots, n-1 \ , \quad (3.1)$$

$$I_n = \{n-2,n-1\} \quad \text{for} \quad d_n .$$

The $O(h^2)$ approximations will give an $O(h^3)$ error bound for the rational quadratic method. The weights associated with the formulae are given in
terms of the interval lengths as

\[ \alpha_{1,2} = 1 + \frac{h_1}{h_2}, \quad \alpha_{1,3} = -\frac{h_1}{h_2} \quad \text{for } d_1, \]

\[ \alpha_{i,i-1} = \frac{h_i}{(h_{i-1} + h_i)}, \quad \alpha_{i,i+1} = \frac{h_{i-1}}{(h_{i-1} + h_i)} \quad \text{for } d_i, \quad i = 2, \ldots, n-1 \quad (3.2) \]

\[ \alpha_{n,n-1} = 1 + \frac{h_{n-1}}{h_{n-2}}, \quad \alpha_{n,n-2} = -\frac{h_{n-1}}{h_{n-2}} \quad \text{for } d_n \]

The arithmetic means for \( d_1 \) and \( d_n \) can be negative, such values being replaced by zero in the rational quadratic scheme. The geometric and harmonic means are all non-negative, the harmonic means having the simplified forms

\[ d_1 = \frac{\Delta_{1,2}}{\Delta_{1,3}} \Delta_{2,3}, \]

\[ d_i = \frac{\Delta_{i,i-1}}{\Delta_{i,i+1}} \Delta_{i,i+1}, \quad i = 2, \ldots, n-1, \quad (3.3) \]

\[ d_n = \frac{\Delta_{n,n-1}}{\Delta_{n,n-2}} \Delta_{n-1,n-2} \]

This form for \( d \) is one used in Gregory and Delbourgo (1982) although there its harmonic mean formulation was not recognized. If \( d_1 \) or \( d_n \) become infinite in the harmonic case they are replaced by a large finite value.

The results of using the derivative parameters defined above, in the rational quadratic scheme, are shown in Figures 1, 2 and 3. It can be seen that the geometric and harmonic settings give better results than those which use the arithmetic form. The geometric setting probably gives the best result for the Fritsch-Carlson data whilst the harmonic setting is better for the other examples.
3.3 $O(h^4)$ interpolation methods

Let $m = 4$. Then $O(h^4)$ derivative approximations are given by the choice

$$I_i = \{i-2, i-1, i+1, i+2\} \text{ for } d_i, \quad i = 3, \ldots, n-2.$$  \hfill (3.4)

These will result in $O(h^4)$ error bounds for the rational quadratic method provided $d_1, d_2, d_{n-1}$ and $d_n$ are given with at least $O(h^3)$ accuracy. We prefer the use of the $O(h^4)$ approximations, which are symmetric about $x_i$, rather than the use of the unsymmetric $O(h^3)$ forms based on

$I_i = \{i-1, i+1, i+2\}, \quad i = 2, \ldots, n-2$ or $I_i = \{i-2, i-1, i+1\}, \quad i = 3, \ldots, n-1.$

This is confirmed in practice, for each of the three data sets, by results which are not shown here. In particular, near the end where there is a change between the two types of $O(h^3)$ settings, the behaviour of the interpolants was found to be poor.

Expressions for the weights can easily be obtained from (2.5) in terms of the interval spacings $h_i$. For brevity we do not quote these here, but note that $\alpha_{1,1-2}$ and $\alpha_{1,1+2}$ are negative and hence the arithmetic mean can give negative values. The geometric mean, as always, is positive and it can be proved that the harmonic mean is also positive.

It is sufficient to use $O(h^3)$ conditions near the ends, where (3.4) cannot be applied, and these are given by

$$I_1 = \{2, 3, 4\} \text{ for } d_1, \quad I_2 = \{1, 3, 4\} \text{ for } d_2, \quad I_n = \{n-3, n-2, n-1\} \text{ for } d_n, \quad I_{n-1} = \{n-3, n-2, n\} \text{ for } d_{n-1}.$$  \hfill (3.5)

Here the arithmetic and harmonic settings for $d_1$ and $d_n$ could give negative values. The arithmetic setting for $d_2$ and $d_{n-1}$ could also be negative but the geometric and harmonic forms are positive.

Figures 4, 5 and 6 show the results of using the derivative parameters of this section in the rational quadratic scheme. Here, the harmonic
settings seem to give the best results, with the arithmetic values again providing the poorest curves. In fact some of the graphs compare unfavourably with those given by the derivative parameters of the previous subsection, although this is not unexpected since the data sets do not exhibit the smoothness conditions needed for $O(h^4)$ convergence. In the next subsection we check the theoretical behaviour of the errors on the smooth test function $f(x) = \exp(x)$.

### 3.4 Test problem $f(x) = \exp(x)$

Tables 3 and 4 show the results of applying the $O(h^3)$ and $O(h^4)$ interpolation methods to $f(x) = \exp(x)$ on $[0,1]$. The derivative settings are those described above except that the exact end conditions $d_1 = 1$ and $d = \exp(1)$ are used. The knots are taken to be equally spaced with four choices of interval length, $h = 0.2$, 0.1, 0.05, and 0.025 respectively. The tables give the uniform norm errors $||f - s||_\infty$ on $[0,1]$ and the ratios of the errors confirm the expected $O(h^3)$ and $O(h^4)$ error bounds. Both the geometric and harmonic settings have given consistently smaller error norms than those given by the arithmetic settings for this example.

<table>
<thead>
<tr>
<th></th>
<th>Error $E_1$ (h=0.2)</th>
<th>Error $E_2$ (h=0.1)</th>
<th>Error $E_3$ (h=0.05)</th>
<th>Error $E_4$ (h=0.025)</th>
<th>$E_1/E_2$</th>
<th>$E_2/E_3$</th>
<th>$E_3/E_4$</th>
</tr>
</thead>
<tbody>
<tr>
<td>Arithmetic</td>
<td>0.4620×10^{-3}</td>
<td>0.6226×10^{-4}</td>
<td>0.8081×10^{-5}</td>
<td>0.1029×10^{-5}</td>
<td>7.42</td>
<td>7.70</td>
<td>7.85</td>
</tr>
<tr>
<td>Geometric</td>
<td>0.1217×10^{-3}</td>
<td>0.1597×10^{-4}</td>
<td>0.2046×10^{-5}</td>
<td>0.2589×10^{-6}</td>
<td>7.62</td>
<td>7.81</td>
<td>7.90</td>
</tr>
<tr>
<td>Harmonic</td>
<td>0.2180×10^{-3}</td>
<td>0.3030×10^{-4}</td>
<td>0.3988×10^{-5}</td>
<td>0.5113×10^{-6}</td>
<td>7.19</td>
<td>7.60</td>
<td>7.80</td>
</tr>
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</table>

Table 3. $E - ||f - s||_\infty$, $O(h^3)$ interpolation methods, $f(x) = \exp(x)$
<table>
<thead>
<tr>
<th></th>
<th>Error $E_1$  (h=0.2)</th>
<th>Error $E_2$  (h=0.1)</th>
<th>Error $E_3$  (h=0.05)</th>
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<th>$E_1/E_2$</th>
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<tr>
<td>Arithmetic</td>
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<td>$0.1498 \times 10^{-7}$</td>
<td>14.34</td>
<td>15.14</td>
<td>15.56</td>
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<tr>
<td>Geometric</td>
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<td>$0.2736 \times 10^{-8}$</td>
<td>15.29</td>
<td>15.65</td>
<td>15.82</td>
</tr>
<tr>
<td>Harmonic</td>
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<td>$0.6557 \times 10^{-6}$</td>
<td>$0.4258 \times 10^{-7}$</td>
<td>$0.2713 \times 10^{-8}$</td>
<td>14.83</td>
<td>15.40</td>
<td>15.69</td>
</tr>
</tbody>
</table>

Table 4. \( E = \| f - s \|_{\infty}, \) \( 0(h^4) \) interpolation methods, \( f(x) = \exp(x) \)

4. Conclusion

Given a monotonic data set, a \( C^1 \) monotonic interpolant can be constructed using piecewise rational quadratic interpolation. The theory and results indicate that if the derivative parameters of the scheme are to be calculated from explicit formulae, then the geometric or harmonic approximations of this paper should be used. In particular, for most practical purposes, the formulae giving the \( 0(h^3) \) interpolation methods described in sub-section 4.2 should be adequate.

References


Figure 1. Interpolation methods: Fritsch-Carlson data.

(i) Arithmetic

(ii) Geometric

(iii) Harmonic
Figure 2. 0(h\(^3\)) interpolation methods, Preuss data.
Figure 3. $O(h^3)$ interpolation methods, quarter circle data.

(i) Arithmetic

(ii) Geometric

(iii) Harmonic
Figure 4. $O(h^2)$ interpolation methods, Fritsch-Carlson data.
Figure 5. \(0(1^{-4})\) interpolation methods. Preuss
Figure 6. $O(h^4)$ interpolation methods, quarter circle data.

(i) Arithmetic

(ii) Geometric

(iii) Harmonic