TR/07/84 July 1984

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), $i = 1,\ldots,n$, denote the data, where $x_1 < x_2 < \ldots < x_n$, and assume that $f_1 \leq f_2 \leq \ldots \leq f_n$ (monotonic increasing data). Then derivative parameters d_i, $i = 1,\ldots,n$, are to be determined at the knots x_i, $i = 1,\ldots,n$, which satisfy the necessary monotonicity conditions $d_i \geq 0$, $i = 1,\ldots,n$. The interpolation method then constructs a monotonic piecewise rational quadratic function $s(x)$ such that

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

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

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

where

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

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

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

$$| f(x) - s(x) \leq \max_i | f_i^{(1)} - d_i | 0(h) + 0(h^4) \;, \tag{1.4}$$

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 $f_i^{(1)} = f^{(1)}(x_i)$. 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 $0(h^3)$ accurate derivative parameters d_i, $i = 2,\ldots,n-1$, 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 $0(h^3)$ non-negative approximations to them are required in order to preserve the optimal $0(h^4)$ accuracy of the rational spline.

2. The Derivative Formulae

Let I_i denote an index set of m values $j \in \{1,\ldots,n\}$, $j \neq i$, 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 $0(h)$ derivative approximations to $f_i^{(1)}$. 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 $f_i^{(1)} - d_i = 0(h^m)$ for each of the following generalized arithmetic, geometric and harmonic means:

$$d_i \sum_{j \in I_i} \alpha_{i,j} \Delta_{i,j} , \tag{2.1}$$

$$d_i = \prod_{j \in I_i} \Delta_{i,j}^{\alpha_{i,j}}, \qquad (2.2)$$

$$d_i = 1 \Big/ \sum_{j \in I_i} \alpha_{ij}/\Delta_{i,j} \quad , \qquad (2.3)$$

where

$$\Delta_{i,j} = (f_j - f_i)/(x_j - x_i), \qquad (2.4)$$

$$\alpha_{i,j} = \prod_{\substack{k \in I_i \\ k \neq j}} \left(\frac{x_k - x_i}{x_k - x_j} \right) \qquad (2.5)$$

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 a $\Delta_{i,j} = 0$, since monotonicity implies $s(x)$ = constant between x_i and x_j and hence $d_i = 0$. Thus if $\lim d_i \neq 0$ as a $\Delta_{i,j} \to 0$ 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.

<u>Lemma 2.1.</u> Let I denote an index set of m positive integers and let ϵ_j, $j \in I$, be m distinct non-zero values. Then the linear system in the

unknowns α_j, defined by

$$\sum_{j\in I} \alpha_j = 1 \ , \quad \sum_{j\in I} \varepsilon_j^k \ \alpha_j = 0 \ , \quad k = 1,\dots\dots\ ....,\ m-1 \qquad , \tag{2.6}$$

has the unique solution

$$\alpha_{i,\,j} = \mathop{\pi}_{\substack{k\,\in\, I \\ k\,\neq\, j}} \left(\frac{\varepsilon_k}{\varepsilon_k - \varepsilon_j} \right) \ , \quad j \in I \ . \tag{2.7}$$

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

$$\begin{bmatrix} 1 & 1 & \dots & 1 \\ \varepsilon_1 & \varepsilon_2 & \dots & \varepsilon_m \\ . & . & \dots & . \\ . & . & \dots & . \\ \varepsilon_1^{m-1} & \varepsilon_2^{m-2} & \dots & \varepsilon_m^{m-1} \end{bmatrix} \begin{bmatrix} \alpha_1 \\ \alpha_2 \\ . \\ . \\ \alpha_m \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ . \\ . \\ 0 \end{bmatrix} \tag{2.8}$$

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

$$V(\varepsilon_1,\dots\dots\ \varepsilon_m) = \mathop{\pi}_{p>q}^{m} (\varepsilon_p - \varepsilon_q)$$

and (2.8) has the unique solution

$$\alpha_j = \frac{V(\varepsilon_1,\dots\dots,\ 0,\dots\dots,\ \varepsilon_m)}{V(\varepsilon_1,\dots\dots,\ \varepsilon_j,\dots\dots,\ \varepsilon_m)} = \mathop{\pi}_{\substack{k=1 \\ k\neq j}}^{m} \left(\frac{\varepsilon_k}{\varepsilon_k - \varepsilon_j} \right)$$

<u>Lemma 2.2</u> Let $\lambda > 0$ and $\lambda_j > 0$ be given such that

$$\lambda_j = \lambda + \sum_{k=1}^{m-1} b_k \ \varepsilon_j^k + 0\,(\varepsilon^m) \ , \quad j \in I \ , \tag{2.9}$$

where b_k are constants (independent of j), $\varepsilon = \max|\varepsilon_j|$ and the ε_j satisfy the hypotheses of Lemma 2.1. Then the generalized arithmetic, geometric and harmonic means defined by

$$A = \sum_{j\in I} \alpha_j \lambda_j \ , \quad G = \sum_{j\in I} \lambda_j^{\alpha_j} \ , \quad H = 1 \Big/ \sum_{j\in I} \alpha_j/\lambda_j \tag{2.10}$$

are all $0(\varepsilon^m)$ approximations to λ, where the α_j are defined by (2.7) of Lemma 2.1.

<u>Proof</u> (i) Substituting (2.9) in the definition of the arithmetic mean gives

$$A \sum_{j\in I} \alpha_j [\lambda + 0(\varepsilon^m)] + \sum_{k=1}^{m-1} b_k \sum_{j\in I} \alpha_j \varepsilon_j^k \ .$$

Thus $A = \lambda + 0(\varepsilon^m)$ for α_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

$$\begin{aligned} \text{Log } G &= \sum_{j\in I} \alpha_j \log \lambda_j \\ &= \sum_{j\in I} \alpha_j \left[\log\lambda + \log\left\{ 1 + \sum_{k=1}^{m} \lambda^{-1} b_k \varepsilon_j^k + 0(\varepsilon^m) \right\} \right] \\ &= \sum_{j\in I} \alpha_j \log\lambda + \sum_{j\in I} \alpha_j \left\{ \sum_{k=1}^{m} c_k \varepsilon_j^k + 0(\varepsilon^m) \right\} \end{aligned}$$

wherethe c_k are constants, obtained by collecting terms of a power series expansion of the second logarithmic term. Thus log G - log $\lambda + 0(\varepsilon^m)$, for et. satisfying (2.6) and hence $G = \lambda + 0(\varepsilon^m)$.

(iii) Noting that $\lambda \neq 0$, we take the reciprocal of the harmonic mean and substitute (2.9) to give

$$H^{-1} = \lambda^{-1} \sum_{j \in I} \alpha_j \left[1 + \sum_{k=1}^{m-1} \lambda^{-1} b_k \varepsilon_j^k + 0(\varepsilon^m) \right]^{-1}$$

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

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 α_j. satisfying (2.6) and hence $H = \lambda + 0(\varepsilon^m)$.

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 $\lambda < 0$, $\lambda_j.<0$, $j \in 1$, with the geometric mean now being defined by

$$G = - \pi_{j \in I} (-\lambda_j)^{\alpha j}$$

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

$$\Delta_{i,j} = f_i^{(1)} + \sum_{k=1}^{m-1} b_{i,k} \varepsilon_{i,j}^k + 0(\varepsilon_{i,j}^m) \quad , \quad j \in I_i \ , \tag{2.11}$$

where $b_{i,k} = f_i^{(k+1)}/(k+1)!$ and $\varepsilon_{ij} = x_j - x_i$. 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° arguments over a quarter circle and is distinguished by the difficulty of an infinite gradient at an end point.

X	7.99	8.09	8.19	8.7	9.2	10	12	15	20
y	0	2.7629×10^{-5}	$4.37498\text{x}10^{-2}$	0.169183	0.469428	0.943740	0.998636	0.999919	0.999994

Table 1, Fritsch-Carlson data.

X	22	22.5	22.6	22.7	22.8	22.9	23	23.1	23.2	23.3	23.4	23.5	24
y	523	543	550	557	565	575	590	620	860	915	944	958	986

Table 2. Pruess data.

3.2 $Q(h^3)$ interpolation methods

Let m = 2. Then equations (2.1) -(2.3) give $0(h^2)$ derivative approximations with the following choices of index sets:

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

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

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

The $0(h^2)$ approximations will give an $0(h^3)$ error bound for the rational quadratic method. The weights associated with the formulae are given in terms of the interval lengths as

$$\alpha_{1,2} = 1 + h_1/h_2\ ,\quad \alpha_{1,3} = -h_1/h_2 \qquad \text{for } d_1\ ,$$

$$\alpha_{i,i-1} = h_i/(h_{i-1}+h_i)\ ,\quad \alpha_{i,i+1} = h_{i-1}/(h_{i-1}+h_i) \quad \text{for } d_i\ ,\ i=2,\ldots,n-1\ , \qquad (3.2)$$

$$\alpha_{n,n-1} = 1 + h_{n-1}/h_{n-2}\ ,\quad \alpha_{n,n-2} = -h_{n-1}/h_{n-2} \qquad \text{for } d_n$$

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

$$d_1 = \Delta_{1,2}\ \Delta_{1,3}/\Delta_{2,3}\ ,$$

$$d_i = \Delta_{i,i-1}\ \Delta_{i,i+1}/\Delta_{i-1,i+1}\ ,\quad i = 2,\ldots,n-1\ , \qquad (3.3)$$

$$d_n = \Delta_{n,n-1}\ \Delta_{n,n-2}/\Delta_{n-1,n-2}$$

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 <u>$0(h^4)$ interpolation methods</u>

Let $m = 4$. Then $0(h^4)$ derivative approximations are given by the choice

$$I. = \{i-2, i-1, i+1, i+2\} \quad \text{for} \quad d_i \quad , \quad i = 3, \ldots, n-2 \quad . \tag{3.4}$$

These will result in $0(h^4)$ error bounds for the rational quadratic method provided d_1, d_2, d_{n-1} and d_n are given with at least $0(h^3)$ accuracy. We prefer the use of the $0(h^4)$ approximations, which are symmetric about x_i, rather than the use of the unsymmetric $0(h^3)$ forms based on I_i - $\{i-1, i+1, i+2\}$, $i = 2, \ldots, n-2$ or $I_i = \{i-2, i-1, i+1\}$, $i = 3, \ldots, n-1$. 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 $0(h^3)$ 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 $0(h^3)$ conditions near the ends, where (3.4) cannot be applied, and these are given by

$$\begin{array}{llll} I = \{2,3,4\} & \text{for } d_1 \; , & I_2 = (1,3,4\} & \text{for } d_2 \; , \\ I_n = \{n-3, n-2, n-l\} & \text{for } d_n \; , & I_{n-1} = \{n-3, n-2, n\} & \text{for } d_{n-1} \; . \end{array} \tag{3.5}$$

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 $0(h^4)$ convergence. In the next subsection we check the theoretical behaviour of the errors on the smooth test function $f(x) = \exp(x)$.

3.4 <u>Test problem f(x) =exp(x)</u>

Tables 3 and 4 show the results of applying the $0(h^3)$ and $0(h^4)$ 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 $0(h^3)$ and $0(h^4)$ error bounds. Both the geometric and harmonic settings have given consistently smaller error norms than those given by the arithmetic settings for this example.

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

Table 3. $E - \| f - s \|_\infty$, $0(h^3)$ interpolation methods, $f(x) = \exp(x)$

	Error E_1 (h=0.2)	Error E_2 (h=0.1)	Error E_3 (h=0.05)	Error E_4 (h=0.025)	E_1/E_2	E_2/E_3	E_3/E_4
Arithmetic	0.5058×10^{-4}	0.3528×10^{-5}	0.2331×10^{-6}	0.1498×10^{-7}	14.34	15.14	15.56
Geometric	0.1036×10^{-4}	0.6774×10^{-6}	0.4329×10^{-7}	0.2736×10^{-8}	15.29	15.65	15.82
Harmonic	0.9724×10^{-5}	0.6557×10^{-6}	0.4258×10^{-7}	0.2713×10^{-8}	14.83	15.40	15.69

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.

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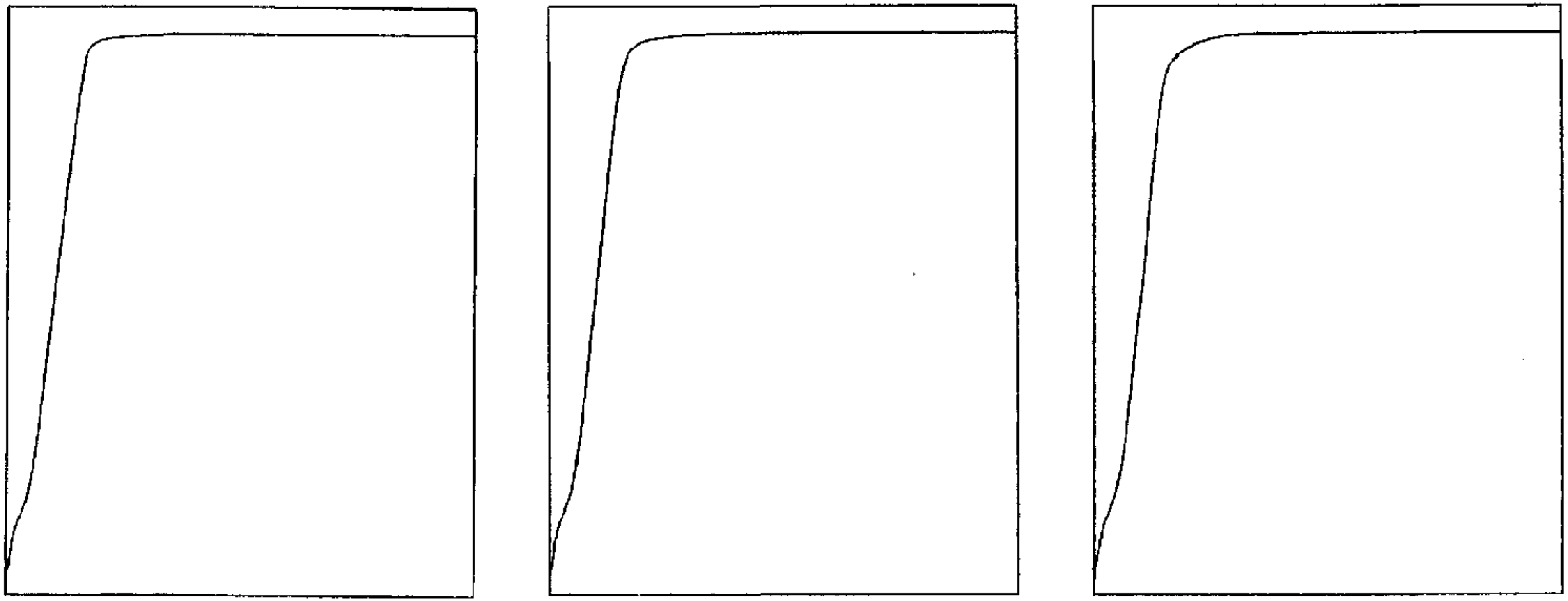
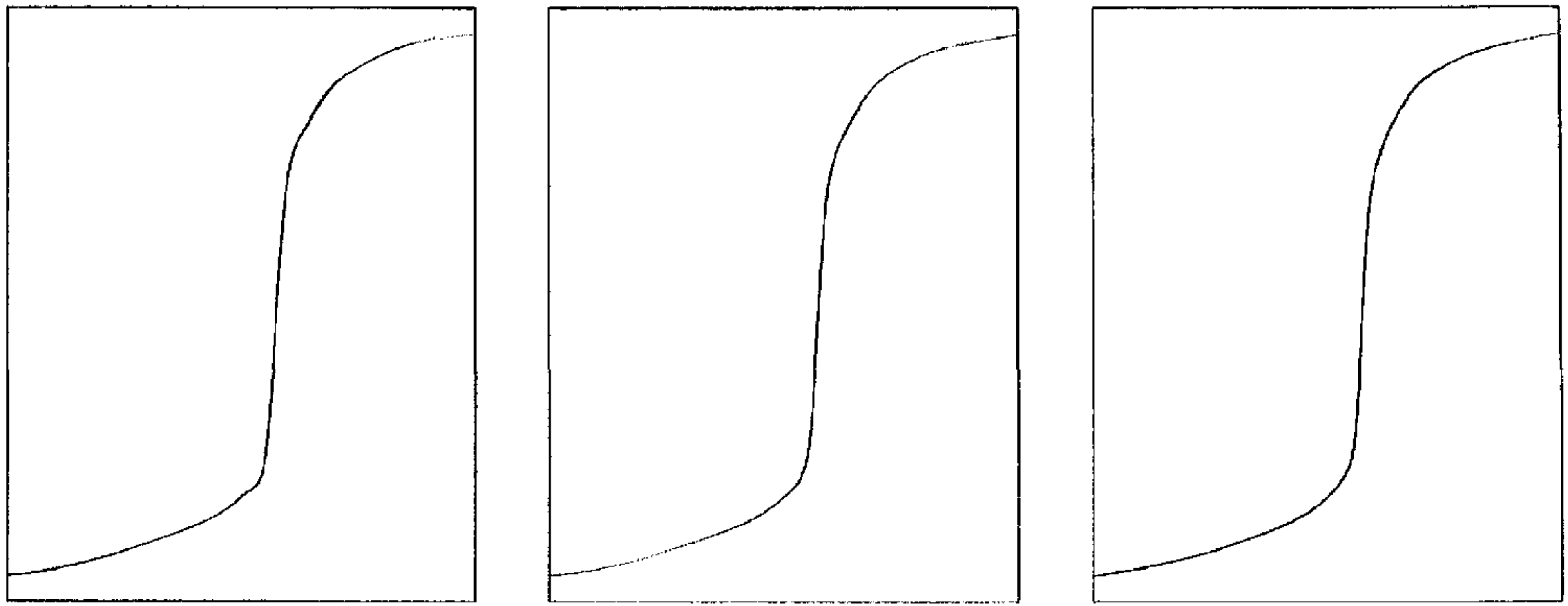


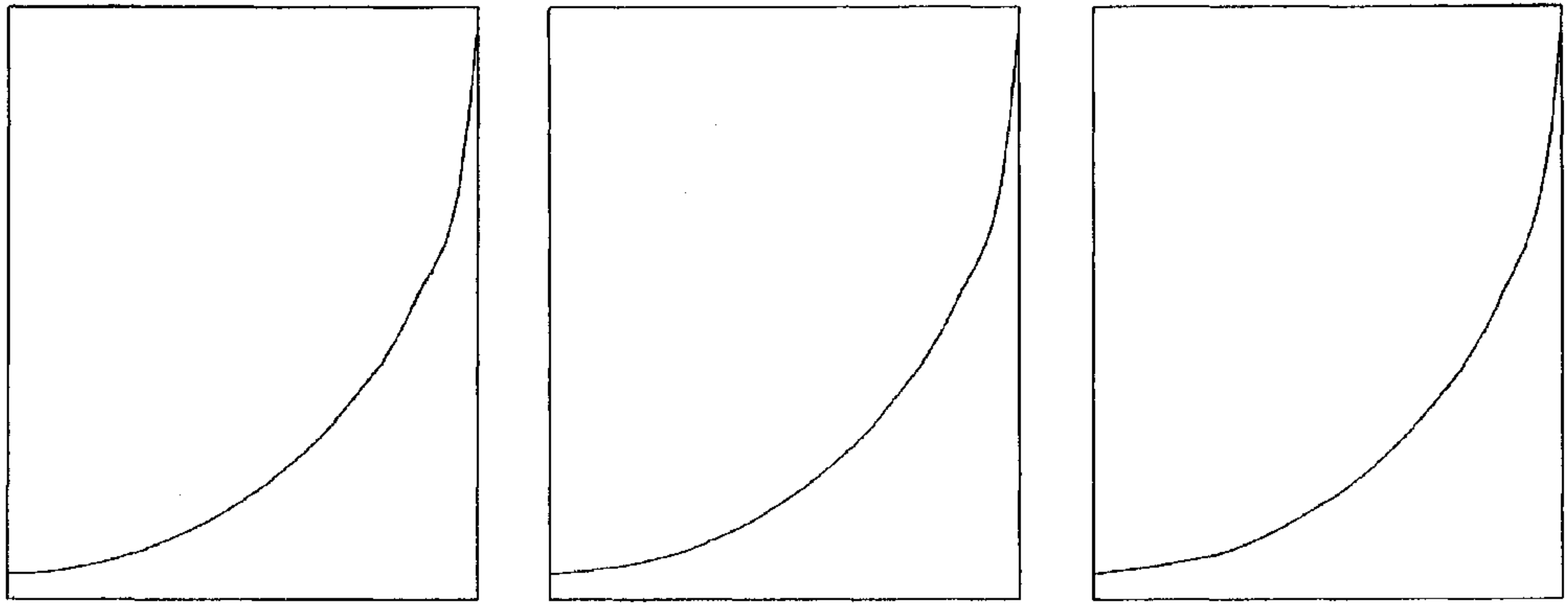
(i) Arithmetic (ii) Geometric (iii) Harmonic

Figure 1. $0(h^3)$ interpolation methods, Fritsch-Carlson data.



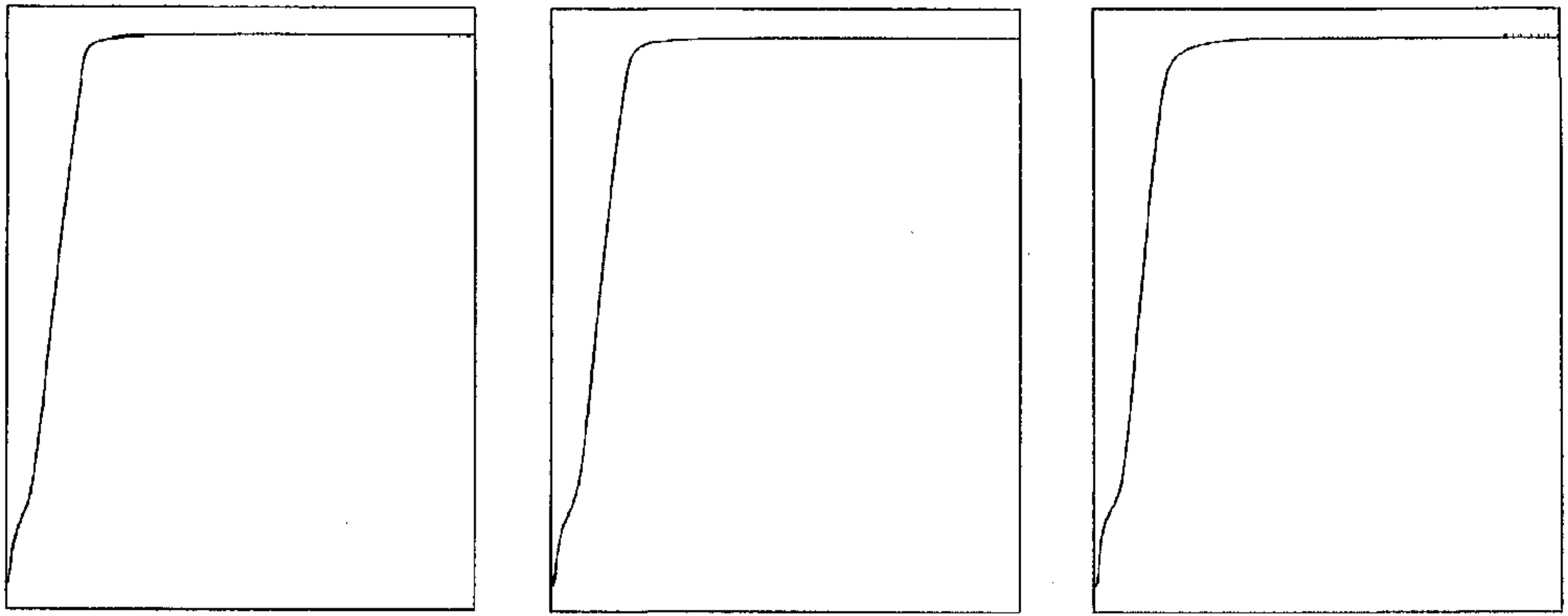
(i) Arithmetic (ii) Geometric (iii) Harmonic

Figure 2. $0(h^3)$ interpolation methods, Preuss data.



(i) Arithmetic (ii) Geometric (iii) Harmonic

Figure 3. $0(h^3)$ interpolation methods, quarter circle data.



(i) Arithmetic (ii) Geometric (iii) Harmonic

Figure 4. $0(h^4)$ interpolation methods, Fritsch-Carlson data.

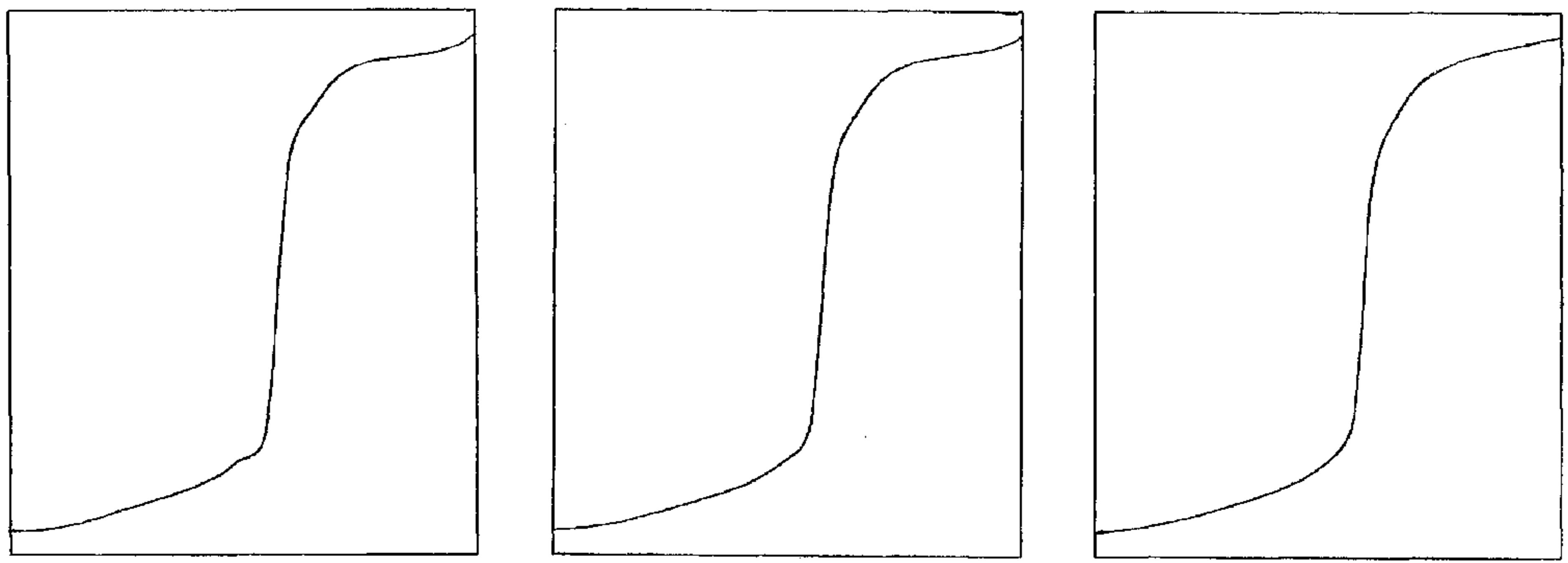
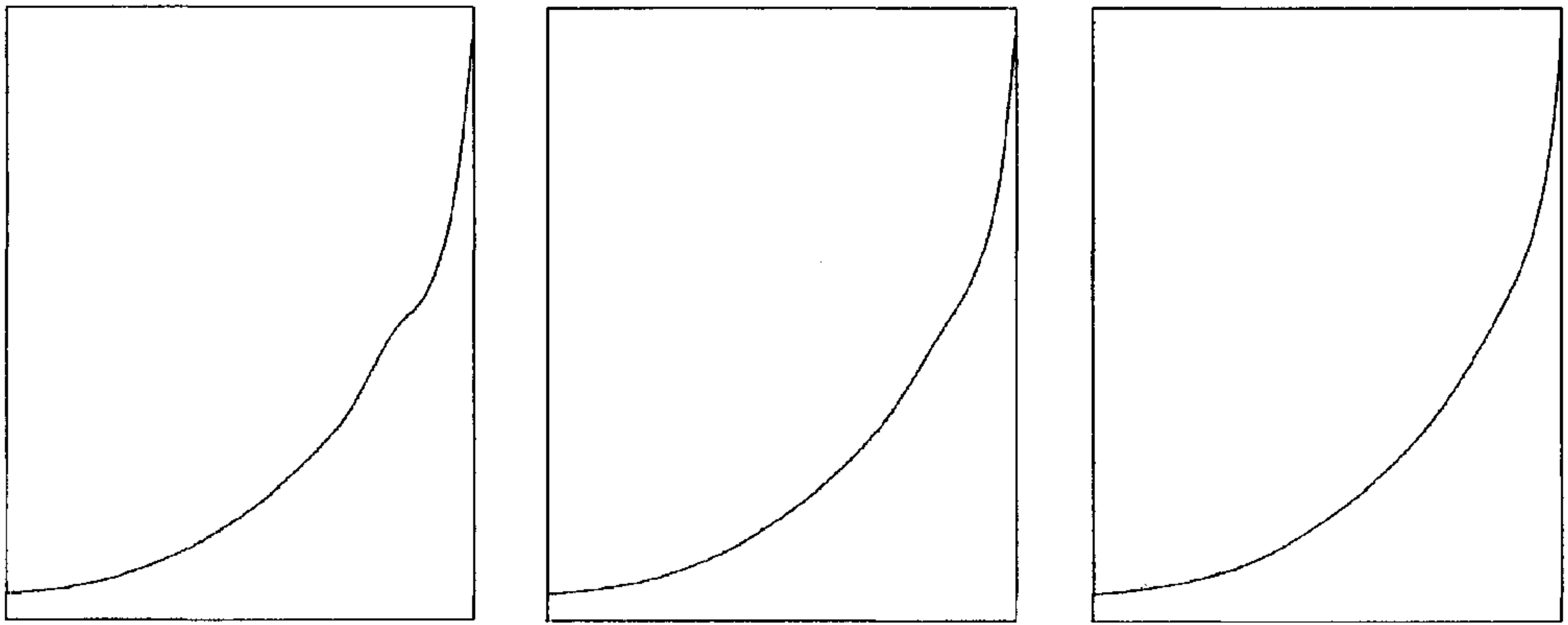


Figure 5. $0(h^4)$ interpolation methods, Preuss



(i) Arithmetic (ii) Geometric (iii) Harmonic

Figure 6. $0(h^4)$ interpolation methods, quarter circle data.