

An error term and uniqueness for Hermite–Birkhoff interpolation involving only function values and/or first derivative values

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Abstract

This paper discusses various aspects of Hermite–Birkhoff interpolation that involve prescribed values of a function and/or its first derivative. An algorithm is given that finds the unique polynomial satisfying the given conditions if it exists. A mean value type error term is developed which illustrates the ill-conditioning present when trying to find a solution to a problem that is close to a problem that does not have a unique solution. The interpolants we consider and the associated error term may be useful in the development of continuous approximations for ordinary differential equations that allow asymptotically correct defect control. Expressions in the algorithm are also useful in determining whether certain specific types of problems have unique solutions. This is useful, for example, in strategies involving approximations to solutions of boundary value problems by collocation.

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1. Introduction

This paper discusses Hermite–Birkhoff interpolation for the case where the given information contains function values and/or first derivative values at given knots. Specifically, we give a simple algorithm to compute the unique interpolant, if it exists, then present a mean value type error expression, and finally give some results concerning uniqueness. This case arises in many applications. For example, it may arise when using collocation to solve two-point boundary value problems (see [7,9]). Another example arises in the numerical solution of ordinary differential equations with defect control when using Runge–Kutta methods (see [8,4]).

As Higham [8] points out, there is a well-known error expression in the case of Hermite interpolation, but not for Hermite–Birkhoff interpolation. Birkhoff [2] (see also [13, p. 84]), in his important paper in 1906, showed an error expression for the general Hermite–Birkhoff problem. However, after this paper, research centered on the difficult question of what knots produced a unique solution and not on the error involved. The error expression developed here specifically involves only the case of function and/or first derivative values. It does not extend simply to cases where

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higher order derivatives are involved. However, in its final form in Section 3, we present an expression not too much more complicated than the well-known error expression for Hermite interpolation. Although the expression does involve a matrix, the dimension of this matrix is in many cases much smaller than the dimension of the determinant involved in the expression given in Birkhoff [2]. A potential use of this error expression is in the development of continuous approximations to ordinary differential equations which would allow asymptotically correct defect control. Another use of the error expression is in Finden [7] where it is used to show the accuracy of certain interpolation schemes used to improve collocation solutions in the numerical solution of boundary value problems. This error expression illustrates the ill-conditioning present when trying to find the solution to a Hermite–Birkhoff problem when it is close to a problem that does not have a unique solution.

Section 2 discusses a method for the calculation of the unique interpolant. A key part of this method involves material similar to that developed by Fiala [6] where only the case involving function values or first derivative values specified at a knot is discussed. We will extend this to the case where both function values and/or first derivative values are given at certain knots. We show some of the details here since they are important in Section 3 where the error expression is developed. Section 4 gives a simple example that illustrates the method and the error expression and a second example that illustrates the error expression.

Section 5 discusses how material developed in Section 2 can be used to determine whether there is a unique solution to the problem for certain choices of knots. Some of these cases give some guidelines when choosing the Hermite–Birkhoff interpolation used in Runge–Kutta defect control in Higham [8]. Information in this section also helps in choosing a strategy that uses Hermite–Birkhoff interpolation to improve solutions to boundary value problems obtained using collocation (see [7,9,16]).

We begin with a brief discussion on Hermite–Birkhoff interpolation in general. Let us assume that we are given $n + 1$ specified values $f^{(j)}(\sigma_i) = y_i^j$ for some function $f(x)$. We wish to find the unique polynomial, $Q_n(x)$, if it exists, that satisfies $Q_n^{(j)}(\sigma_i) = y_i^j$. There are numerous papers, including [1,3,5,10,12,14,15,17–19], that discuss the existence of such a polynomial. A thorough discussion and extensive bibliography on the general topic is given in *Birkhoff Interpolation* [13]. For this introduction we use the common notation found (for example) in Mühlbach [14].

We define an index set $e = \{(i, j) | y_i^j \text{ is specified}\}$. We define a $w \times (n + 1)$ incidence matrix $E = [e_{ij}]_{j=0, \dots, n}^{i=1, \dots, w}$, with $w \leq n + 1$, where the element $e_{ij} = 1$ if $(i, j) \in e$. Otherwise $e_{ij} = 0$. We let the set of knots, σ_i , satisfy $\sigma_1 < \sigma_2 < \sigma_3 < \dots < \sigma_w$. We say that E is unconditionally poised if a unique $Q_n(x)$ exists for any set of knots. E is conditionally poised if $Q_n(x)$ exists only for certain sets of knots.

Some well-known examples of interpolation where E is unconditionally poised are Lagrange interpolation, where $w = n + 1$ and only $e_{i,0} = 1$ for each row; Taylor interpolation, where E has only one row with all elements equal to one; and Hermite interpolation where $e_{ij} = 1$ implies that $e_{i,j-1} = 1$ for $j = 1, \dots, n$. However, a simple complete characterization of poised matrices is not known. The matrix

$$E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix} \quad (1)$$

is conditionally poised since a unique $Q_n(x)$ does not exist for $\sigma_2 = (\sigma_1 + \sigma_3)/2$ but does exist for any other σ_2 . The matrix

$$E = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 0 \end{bmatrix} \quad (2)$$

is unconditionally poised. To check these examples we examine the determinant defined in (8) in Section 2. For (1) this determinant is equal to $(\sigma_3 - \sigma_1)(\sigma_3 + \sigma_1 - 2\sigma_2)$. For (2) this determinant is equal to $2(\sigma_3 - \sigma_2)$.

There are many conditions on the matrix, E , that help determine whether it is poised or not (see the bibliography in *Birkhoff Interpolation* [13]). Some of these conditions can be described by the following properties of E . By $m_j = \sum_{i=1}^w e_{ij}$, $j = 0, \dots, n$, we denote the number of ones in column j . By $M_j = \sum_{i=0}^j m_i$, $j = 0, \dots, n$, we denote the number of ones in columns 0 through j . We say that E satisfies the Polya-condition if and only if $M_j \geq j + 1$, for $j = 0, \dots, n$. We have

Theorem 1 (Schoenberg [17]). *A necessary condition for E to be poised for some set of knots is that E satisfy the Polya-condition.*

A row i of E has an (i, j) -sequence of length μ if there is a j such that $e_{i,j-1} = 0$, $e_{ij} = e_{i,j+1} = \dots e_{i,j+\mu-1} = 1$ and $e_{i,j+\mu} = 0$. It is an odd or even sequence depending on whether μ is odd or even. We say an (i, j) -sequence is supported if and only if there are rows i_1 and i_2 , where $i_1 < i$ and $i_2 > i$, that contain a one in a column numbered less than j . The second row of the matrix in (1) has an odd supported $(2,1)$ -sequence. The matrix in (2) has no supported sequences. With these definitions we have:

Theorem 2 (Atkinson and Sharma [1]). *If E satisfies the Polya-condition and has no odd supported sequences, then E is poised.*

Also

Theorem 3 (Schoenberg [17]). *If E satisfies the Polya-condition and has only Hermite data in rows two through $w - 1$, then E is poised.*

These are but a small sample of the results for the general problem of Hermite–Birkhoff interpolation. However, the specific case of prescribed function values and/or first derivative values arises often in practice and so we now restrict ourselves to this case. This will allow us to say something about the selection of knots for which a conditionally poised E gives a unique solution or not as the case may be. For this case the $w \times (n + 1)$ incidence matrix E has the property that for each row, i , we have $e_{i,0} + e_{i,1} = 1$ or 2 and $e_{i,j} = 0$ for $j = 2, \dots, n$. Note that $w = n + 1$ for the case that Fiala [6] discusses, but for our case we have $w \leq n + 1$.

2. The case of function and/or first derivative values

We separate the knots into three groups, $\{t_i\}$, $\{x_i\}$ and $\{s_i\}$, such that we know the function values $f(t_i)$, $1 \leq i \leq k$, we know the first derivative values $f'(x_i)$, $1 \leq i \leq m$, and we know the function and first derivative values $f(s_i)$ and $f'(s_i)$, $1 \leq i \leq l$ for some function $f : \mathfrak{R} \rightarrow \mathfrak{R}$. Our problem is to find the interpolating polynomial $Q_n(x) = a_0 + a_1x + \dots + a_nx^n$ that satisfies the conditions

$$f(t_i) = Q_n(t_i), \quad i = 1, \dots, k, \quad (3)$$

$$f'(x_i) = Q'_n(x_i), \quad i = 1, \dots, m, \quad (4)$$

and

$$f(s_i) = Q_n(s_i), \quad f'(s_i) = Q'_n(s_i), \quad i = 1, \dots, l, \quad (5)$$

where $n = k + m + 2l - 1$. We assume that each of the t_i , each of the x_i and each of the s_i are distinct and that $t_i \neq x_j \neq s_r$ for all i, j and r . We let the interval spanned by these values be represented by I . Of course we can solve our problem if we solve the equations, obtained from (3) to (5),

$$\begin{aligned} a_0 + a_1t_i + a_2t_i^2 + \dots + a_nt_i^n &= f(t_i), & i = 1, \dots, k, \\ a_0 + a_1s_i + a_2s_i^2 + \dots + a_ns_i^n &= f(s_i), & i = 1, \dots, l, \\ a_1 + 2a_2x_i + \dots + na_nx_i^{n-1} &= f'(x_i), & i = 1, \dots, m, \\ a_1 + 2a_2s_i + \dots + na_ns_i^{n-1} &= f'(s_i), & i = 1, \dots, l, \end{aligned} \quad (6)$$

for the coefficients a_i , $0 \leq i \leq n$.

Eqs. (6) have a unique solution if and only if the determinant

$$\begin{vmatrix} 1 & t_1 & t_1^2 & \dots & t_1^n \\ & & & & \vdots \\ 1 & t_k & t_k^2 & \dots & t_k^n \\ 1 & s_1 & s_1^2 & \dots & s_1^n \\ & & & & \vdots \\ 1 & s_l & s_l^2 & \dots & s_l^n \\ 0 & 1 & 2x_1 & \dots & nx_1^{n-1} \\ & & & & \vdots \\ 0 & 1 & 2x_m & \dots & nx_m^{n-1} \\ 0 & 1 & 2s_1 & \dots & ns_1^{n-1} \\ & & & & \vdots \\ 0 & 1 & 2s_l & \dots & ns_l^{n-1} \end{vmatrix} \neq 0. \quad (7)$$

For the case, $l = 0$, Eq. (7) becomes

$$\begin{vmatrix} 1 & t_1 & t_1^2 & \dots & t_1^n \\ & & & & \vdots \\ 1 & t_k & t_k^2 & \dots & t_k^n \\ 0 & 1 & 2x_1 & \dots & nx_1^{n-1} \\ & & & & \vdots \\ 0 & 1 & 2x_m & \dots & nx_m^{n-1} \end{vmatrix} \neq 0. \quad (8)$$

If we define the Vandermonde determinant

$$V_j(u_1, u_2, \dots, u_j) = \begin{vmatrix} 1 & u_1 & \dots & u_1^{j-1} \\ 1 & u_2 & \dots & u_2^{j-1} \\ & & & \vdots \\ 1 & u_j & \dots & u_j^{j-1} \end{vmatrix},$$

which can be evaluated as $\prod_{i>j} (u_i - u_j)$, then Fiala [6] points out that we have a unique solution if and only if

$$\frac{\partial^m V_{k+m}(t_1, \dots, t_k, x_1, \dots, x_m)}{\partial x_1 \partial x_2 \dots \partial x_m} \neq 0,$$

which is the same inequality as (8).

We can use (8) to say that we have a unique solution for the case $k = 1$ and $l = 0$ since the resulting determinant can be written as

$$\frac{\partial^m V_{1+m}(t_1, x_1, \dots, x_m)}{\partial x_1 \partial x_2 \dots \partial x_m} = n! V_m(x_1, \dots, x_m) = n! \prod_{i>j} (x_i - x_j) \neq 0.$$

Fiala [6] shows this as well as the fact that for $l = 0$ we have a unique solution if $x_i > t_j$ for all i and j or $x_i < t_j$ for all i and j by appealing to the determinant in (8). Theorem 2 also gives this result. However, using (8) to determine the existence of a unique solution for more complicated problems is not very easy. Solving (6) to obtain the coefficients of $Q_n(x)$ is not recommended since the matrix associated with (7) is ill-conditioned.

We find $Q_n(x)$ in another way by first finding $Q_n(x_i)$, $1 \leq i \leq m$, the corresponding approximations to the function at the points where we know only the first derivatives. We can then use any well-known interpolation scheme such as Hermite interpolation on the data,

$$\{(t_i, f(t_i)), 1 \leq i \leq k\} \cup \{(x_i, Q_n(x_i)), 1 \leq i \leq m\} \cup \{(s_i, f(s_i)), (s_i, f'(s_i)), 1 \leq i \leq l\}.$$

First, we write $Q_n(x)$ in the Hermite form as

$$Q_n(x) = \sum_{j=1}^l H_j(x) f(s_j) + \sum_{j=1}^l \bar{H}_j(x) f'(s_j) + \sum_{j=1}^k G_j(x) f(t_j) + \sum_{j=1}^m K_j(x) Q_n(x_j), \quad (9)$$

where

$$\begin{aligned} H_j(x) &= [1 - (x - s_j) S_j] \frac{\xi_j^2(x) \phi(x) \psi(x)}{\xi_j^2(s_j) \phi(s_j) \psi(s_j)}, \quad 1 \leq j \leq l, \\ \bar{H}_j(x) &= (x - s_j) \frac{\xi_j^2(x) \phi(x) \psi(x)}{\xi_j^2(s_j) \phi(s_j) \psi(s_j)}, \quad 1 \leq j \leq l, \\ G_j(x) &= \frac{\phi_j(x) \psi(x) \xi^2(x)}{\phi_j(t_j) \psi(t_j) \xi^2(t_j)}, \quad 1 \leq j \leq k, \\ K_j(x) &= \frac{\psi_j(x) \phi(x) \xi^2(x)}{\psi_j(x_j) \phi(x_j) \xi^2(x_j)}, \quad 1 \leq j \leq m, \end{aligned} \quad (10)$$

where

$$\begin{aligned} \phi(x) &= \prod_{r=1}^k (x - t_r), \quad \phi_j(x) = \prod_{\substack{r=1 \\ r \neq j}}^k (x - t_r), \quad 1 \leq j \leq k, \\ \psi(x) &= \prod_{r=1}^m (x - x_r), \quad \psi_j(x) = \prod_{\substack{r=1 \\ r \neq j}}^m (x - x_r), \quad 1 \leq j \leq m, \\ \xi(x) &= \prod_{r=1}^l (x - s_r), \quad \xi_j(x) = \prod_{\substack{r=1 \\ r \neq j}}^l (x - s_r), \quad 1 \leq j \leq l, \end{aligned}$$

and

$$S_j = \sum_{i=1}^k \frac{1}{s_j - t_i} + \sum_{i=1}^m \frac{1}{s_j - x_i} + 2 \sum_{\substack{i=1 \\ i \neq j}}^l \frac{1}{s_j - s_i}.$$

Differentiating (9), evaluating the result at x_i , $1 \leq i \leq m$, noting that we require $Q'_n(x_i) = f'(x_i)$, $1 \leq i \leq m$, and noting also that $\psi(x_i) = 0$ for $1 \leq i \leq m$ we obtain

$$\begin{aligned} f'(x_i) &= \sum_{j=1}^l [1 - (x_i - s_j) S_j] \frac{\xi_j^2(x_i) \phi(x_i) \psi'(x_i)}{\xi_j^2(s_j) \phi(s_j) \psi(s_j)} f(s_j) \\ &\quad + \sum_{j=1}^l (x_i - s_j) \frac{\xi_j^2(x_i) \phi(x_i) \psi'(x_i)}{\xi_j^2(s_j) \phi(s_j) \psi(s_j)} f'(s_j) + \sum_{j=1}^k \frac{\phi_j(x_i) \xi^2(x_i) \psi'(x_i)}{\phi_j(t_j) \xi^2(t_j) \psi(t_j)} f(t_j) \\ &\quad + \sum_{j=1}^m \frac{\phi'(x_i) \xi^2(x_i) \psi_j(x_i) + 2\phi(x_i) \xi(x_i) \xi'(x_i) \psi_j(x_i) + \phi(x_i) \xi^2(x_i) \psi'_j(x_i)}{\phi(x_j) \xi^2(x_j) \psi_j(x_j)} Q_n(x_j). \end{aligned} \quad (11)$$

We divide the i th equation by $\phi(x_i)\xi^2(x_i)\psi_i(x_i)$, let $y_j = Q_n(x_j)/\phi(x_j)\xi^2(x_j)\psi_j(x_j)$, note that $\psi'(x_i)/\psi_i(x_i) = 1$ and rearrange to form the linear equations in y_j ,

$$\begin{aligned} \sum_{j=1}^m \left[2 \frac{\xi'(x_i)\psi_j(x_i)}{\xi(x_i)\psi_i(x_i)} + \frac{\phi'(x_i)\psi_j(x_i)}{\phi(x_i)\psi_i(x_i)} + \frac{\psi'_j(x_i)}{\psi_i(x_i)} \right] y_j \\ = \frac{f'(x_i)}{\phi(x_i)\xi^2(x_i)\psi_i(x_i)} - \sum_{j=1}^l \frac{[1 - (x_i - s_j)S_j]f(s_j)}{(x_i - s_j)^2\xi_j^2(s_j)\phi(s_j)\psi(s_j)} \\ - \sum_{j=1}^l \frac{f'(s_j)}{(x_i - s_j)\xi_j^2(s_j)\phi(s_j)\psi(s_j)} - \sum_{j=1}^k \frac{f(t_j)}{(x_i - t_j)\phi_j(t_j)\xi^2(t_j)\psi(t_j)}. \end{aligned} \quad (12)$$

We put these linear equations in the form

$$Ay = b, \quad (13)$$

where $A \in \mathfrak{R}^m \times \mathfrak{R}^m$, $y \in \mathfrak{R}^m$, with elements y_i , $1 \leq i \leq m$, and $b \in \mathfrak{R}^m$. The elements of b are given by the right-hand side of (12). If we note that

$$\begin{aligned} \frac{\psi_j(x_i)}{\psi_i(x_i)} &= \begin{cases} 0 & \text{if } i \neq j, \\ 1 & \text{if } i = j, \end{cases} \quad \frac{\phi'(x_i)}{\phi(x_i)} = \sum_{r=1}^k \frac{1}{x_i - t_r}, \\ \frac{\psi'_j(x_i)}{\psi_i(x_i)} &= \begin{cases} \frac{1}{x_i - x_j} & \text{if } i \neq j, \\ \sum_{\substack{r=1 \\ r \neq i}}^m \frac{1}{x_i - x_r} & \text{if } i = j, \end{cases} \quad \frac{\xi'(x_i)}{\xi(x_i)} = \sum_{r=1}^l \frac{1}{x_i - s_r}, \end{aligned}$$

then from (12) we can write the elements of A as

$$a_{ij} = \begin{cases} \frac{1}{x_i - x_j} & \text{if } i \neq j, \\ 2 \sum_{r=1}^l \frac{1}{x_i - s_r} + \sum_{r=1}^k \frac{1}{x_i - t_r} + \sum_{\substack{r=1 \\ r \neq i}}^m \frac{1}{x_i - x_r} & \text{if } i = j. \end{cases} \quad (14)$$

For the special case $l = 0$, the matrix A has the form

$$A = \begin{bmatrix} \sum_{r=1}^k \frac{1}{x_1 - t_r} + \sum_{\substack{r=1 \\ r \neq 1}}^m \frac{1}{x_1 - x_r} & \cdots & \frac{1}{x_1 - x_m} \\ \frac{1}{x_2 - x_1} & \cdots & \frac{1}{x_2 - x_m} \\ \vdots & \ddots & \vdots \\ \frac{1}{x_m - x_1} & \cdots & \sum_{r=1}^k \frac{1}{x_m - t_r} + \sum_{\substack{r=1 \\ r \neq m}}^m \frac{1}{x_m - x_r} \end{bmatrix}. \quad (15)$$

The interpolation problem has a unique solution if and only if A is non-singular. Although the matrix associated with the determinant in (7) is ill-conditioned, A is generally not ill-conditioned when we have a unique solution unless the set of knots are “close” to a set for which there are either no solutions or multiple solutions. In this case it is the problem itself and not the algorithm that is ill-conditioned. The error expression developed in the next section shows the difficulty of using Hermite–Birkhoff interpolation in such a case.

Having solved the system (13), we can find $Q_n(x_i) = \phi(x_i)\psi_i(x_i)\xi^2(x_i)y_i$ for use in any interpolation scheme or we can use the y_i directly in the fourth sum of (9). Solving (13) requires the solution of a smaller linear system ($m \times m$) than the system (6) which is $(k + m + 2l) \times (k + m + 2l)$. The matrix A in (15) is obtained by Fiala [6] but we have

developed the more general case, (14), here since we explain how to use it to solve the interpolation problem, since it appears in the error term that we develop in the next section and since we use it to discuss uniqueness in Section 5.

3. Error term

The error $E(x)$ at any value x is defined by

$$f(x) = Q_n(x) + E(x), \quad (16)$$

which we write in terms of (9) as

$$f(x) = \sum_{j=1}^l H_j(x) f(s_j) + \sum_{j=1}^l \bar{H}_j(x) f'(s_j) + \sum_{j=1}^k G_j(x) f(t_j) + \sum_{j=1}^m K_j(x) Q_n(x_j) + E(x), \quad (17)$$

where H_j, \bar{H}_j, G_j and K_j are defined by (10). We substitute for $Q_n(x_j)$ in (17) using (16) evaluated at x_j and rearrange terms to get

$$\begin{aligned} f(x) &= \sum_{j=1}^l H_j(x) f(s_j) + \sum_{j=1}^l \bar{H}_j(x) f'(s_j) + \sum_{j=1}^k G_j(x) f(t_j) \\ &\quad + \sum_{j=1}^m K_j(x) f(x_j) - \sum_{j=1}^m K_j(x) E(x_j) + E(x). \end{aligned} \quad (18)$$

Let I be the interval spanned by all the knots. Noting the error for Hermite interpolation

$$\begin{aligned} f(x) &- \sum_{j=1}^l H_j(x) f(s_j) - \sum_{j=1}^l \bar{H}_j(x) f'(s_j) - \sum_{j=1}^k G_j(x) f(t_j) - \sum_{j=1}^m K_j(x) f(x_j) \\ &= L(x) \frac{f^{(n+1)}(c(x))}{(n+1)!}, \end{aligned} \quad (19)$$

where $L(x) = \phi(x)\psi(x)\xi^2(x)$ and $c(x)$ is some value in the interval spanned by I and x , we rewrite (18) to get

$$E(x) = L(x) \frac{f^{(n+1)}(c(x))}{(n+1)!} + \sum_{j=1}^m K_j(x) E(x_j). \quad (20)$$

Assuming f has at least $n+2$ derivatives in the interval I , we differentiate (20) to get

$$E'(x) = \frac{L(x)[f^{(n+1)}(c(x))]' + L'(x)f^{(n+1)}(c(x))}{(n+1)!} + \sum_{j=1}^m K'_j(x) E(x_j).$$

Noting that $E'(x_i) = 0$ and that $L(x_i) = 0$, we obtain the linear system of equations in $E(x_j)$, $1 \leq j \leq m$, given by

$$\sum_{j=1}^m K'_j(x_i) E(x_j) = -L'(x_i) \frac{f^{(n+1)}(c(x_i))}{(n+1)!}.$$

Using (10) and noting that $L'(x_i) = \phi(x_i)\psi_i(x_i)\xi^2(x_i)$, we rewrite this system as

$$\begin{aligned} \sum_{j=1}^m \left[\frac{\phi'(x_i)\psi_j(x_i)\xi^2(x_i) + 2\phi(x_i)\xi(x_i)\xi'(x_i)\psi_j(x_i) + \phi(x_i)\psi'_j(x_i)\xi^2(x_i)}{\phi(x_j)\psi_j(x_j)\xi^2(x_j)} \right] E(x_j) \\ = -\phi(x_i)\psi_i(x_i)\xi^2(x_i) \frac{f^{(n+1)}(c(x_i))}{(n+1)!}, \quad i = 1, \dots, m. \end{aligned}$$

We substitute $\Delta_j = E(x_j)/\phi(x_j)\psi_j(x_j)\xi^2(x_j)$ and divide equation i by $\phi(x_i)\psi_i(x_i)\xi^2(x_i)$. The same calculations using (11) to get (12) are done to get

$$\sum_{j=1}^m \left[2 \frac{\xi'(x_i)}{\xi(x_i)} \frac{\psi_j(x_i)}{\psi_i(x_i)} + \frac{\phi'(x_i)}{\phi(x_i)} \frac{\psi_j(x_i)}{\psi_i(x_i)} + \frac{\psi_j'(x_i)}{\psi_i'(x_i)} \right] \Delta_j = - \frac{f^{(n+1)}(c(x_i))}{(n+1)!}, \quad i = 1, \dots, m.$$

This gives us a system of equations similar to (12) which we write as

$$A\Delta = g, \quad (21)$$

where A is given by (14), $\Delta \in \mathfrak{R}^m$ has components Δ_i , $1 \leq i \leq m$, and $g \in \mathfrak{R}^m$ has components $g_i = -f^{(n+1)}(c(x_i))/(n+1)!$, $1 \leq i \leq m$. With a_{ij}^{-1} the components of A^{-1} , we write $\Delta_i = \sum_{j=1}^m a_{ij}^{-1} g_j$ and so

$$E(x_i) = - \frac{\phi(x_i)\psi_i(x_i)\xi^2(x_i)}{(n+1)!} \sum_{j=1}^m a_{ij}^{-1} f^{(n+1)}(c(x_j)).$$

Substituting this in (20) and using (10) we obtain

$$E(x) = \frac{L(x)f^{(n+1)}(c(x))}{(n+1)!} - \sum_{i=1}^m \phi(x)\psi_i(x)\xi^2(x) \sum_{j=1}^m a_{ij}^{-1} \frac{f^{(n+1)}(c(x_j))}{(n+1)!}$$

and finally

$$E(x) = \frac{\phi(x)\psi(x)\xi^2(x)}{(n+1)!} \left[f^{(n+1)}(c(x)) - \sum_{i=1}^m \frac{1}{x-x_i} \sum_{j=1}^m a_{ij}^{-1} f^{(n+1)}(c(x_j)) \right], \quad (22)$$

where $c(x_i)$, $1 \leq i \leq m$, are in the interval I and $c(x)$ is in the interval spanned by I and x . The values $c(x_i)$ are dependent on all the knots. The value of $c(x)$ depends on all the knots and also x .

The appearance of the elements of A^{-1} in (22) illustrates the problem of finding a solution for a choice of knots that are “close” to a set that does not give a unique solution. In this case we have an almost singular matrix A , giving us large values of a_{ij}^{-1} in the error term.

Perhaps a more useful form of this error term can be obtained in the following way. Let $\max\{f^{(n+1)}(c(x)), f^{(n+1)}(c(x_i)), i = 1, \dots, m\} = f^{(n+1)}(\bar{c})$. Then we have

$$|E(x)| \leq \frac{|\phi(x)\xi^2(x)f^{(n+1)}(\bar{c})|}{(n+1)!} \left[|\psi(x)| + \sum_{i=1}^m \left| \frac{\psi(x)}{x-x_i} \right| \sum_{j=1}^m |a_{ij}^{-1}| \right],$$

giving

$$|E(x)| \leq \frac{|\phi(x)\xi^2(x)f^{(n+1)}(\bar{c})|}{(n+1)!} \left[|\psi(x)| + \|A^{-1}\|_{\infty} \sum_{i=1}^m |\psi_i(x)| \right]. \quad (23)$$

We have an expression similar to (19). The extra term in (23) involves a matrix of dimension m which in many applications will be much smaller than the dimension, $k+m+2l$, of the determinant involved in the error expression given in Birkhoff [2]. Of course, (23) applies only to cases involving only function and/or first derivative values, whereas the expression in Birkhoff [2] applies to the general Hermite–Birkhoff interpolation problem.

4. Examples

We illustrate the algorithm and the error term, (22) with our first example. We take the function $f(x) = x^4 + x$ and form $Q_2(x)$ by specifying that

$$Q_2(0) = f(0), \quad Q_2'(-1) = f'(-1), \quad Q_2'(1) = f'(1).$$

Hence we have $l = 0, k = 1, m = 2, t_1 = 0, x_1 = -1, x_2 = 1, Q_2(0) = 0, Q_2'(-1) = -3$ and $Q_2'(1) = 5$. The matrix A in (15) and its inverse are given by

$$A = \begin{bmatrix} -\frac{3}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{3}{2} \end{bmatrix}, \quad A^{-1} = \begin{bmatrix} -\frac{3}{4} & -\frac{1}{4} \\ \frac{1}{4} & \frac{3}{4} \end{bmatrix}.$$

We have $\phi(x) = x, \phi_1(x) = 1, \psi(x) = x^2 - 1, \psi_1(x) = x - 1$ and $\psi_2(x) = x + 1$, and so we have using the right-hand side of (12)

$$b_1 = \frac{f'(-1)}{\phi(-1)\psi_1(-1)} - \frac{f(0)}{-\phi_1(0)\psi(0)} = -\frac{3}{2}$$

and

$$b_2 = \frac{f'(1)}{\phi(1)\psi_2(1)} - \frac{f(0)}{\phi_1(0)\psi(0)} = \frac{5}{2}.$$

Solving $Ay = b$, we get $y_1 = \frac{1}{2}$ and $y_2 = \frac{3}{2}$. Hence

$$Q_2(-1) = \phi(-1)\psi_1(-1)y_1 = 1 \quad \text{and} \quad Q_2(1) = \phi(1)\psi_2(1)y_2 = 3.$$

Finally, using (9) we have $Q_2(x) = 2x^2 + x$.

Knowing the function $f(x)$ allows us to illustrate (22) by finding the values of $c(x), c(x_1)$ and $c(x_2)$. First, we know $E(x) = f(x) - Q_2(x) = x^4 - 2x^2$. Therefore $E(-1) = -1$ and $E(1) = -1$ and therefore

$$A_1 = \frac{E(-1)}{\phi(-1)\psi_1(-1)} = -\frac{1}{2} \quad \text{and} \quad A_2 = \frac{E(1)}{\phi(1)\psi_2(1)} = -\frac{1}{2}.$$

Since $g_i = -f^{(n+1)}(c(x_i))/(n+1)!$ we have $g_1 = -4c(x_1)$ and $g_2 = -4c(x_2)$ and therefore using (21) we have

$$\begin{bmatrix} -4c(-1) \\ -4c(1) \end{bmatrix} = \begin{bmatrix} -\frac{3}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{3}{2} \end{bmatrix} \begin{bmatrix} -\frac{1}{2} \\ -\frac{1}{2} \end{bmatrix},$$

giving $c(-1) = -\frac{1}{4}$ and $c(1) = \frac{1}{4}$.

To find $c(x)$ we substitute in (22) and obtain

$$x^4 - 2x^2 = \frac{x^3 - x}{6} \left[24c(x) - \frac{3}{x+1} - \frac{3}{x-1} \right],$$

giving $c(x) = x/4$ for any value of $x \neq -1, 0$ or 1 . Hence we have $c(x_1)$ and $c(x_2)$ in I and $c(x)$ in the interval spanned by I and x .

For our second example, we illustrate the error bound (23). Let $f(x) = e^x$, and find $Q_6(x)$ using $t_1 = 0, x_1 = -\frac{1}{2}, x_2 = \frac{1}{2}, s_1 = -1, s_2 = 1$. Hence we have $k = 1, m = 2, l = 2$ and $n = 6$. Using (14) this gives

$$A = \begin{bmatrix} -\frac{1}{3} & -1 \\ 1 & \frac{1}{3} \end{bmatrix}, \quad A^{-1} = \begin{bmatrix} \frac{3}{8} & \frac{9}{8} \\ -\frac{9}{8} & -\frac{3}{8} \end{bmatrix}.$$

Using the right-hand side of (12), we get

$$b_1 = \frac{32}{9} e^{-1/2} + \frac{46}{9} e^{-1} - \frac{26}{27} e - 8, \quad b_2 = \frac{32}{9} e^{1/2} + \frac{38}{27} e^{-1} - \frac{34}{9} e + 8.$$

Solving $Ay = b$ again and then using y we obtain

$$Q_6(-1/2) = \frac{27}{16} + \frac{3}{8} e^{-1/2} + \frac{9}{8} e^{1/2} + \frac{63}{64} e^{-1} - \frac{83}{64} e,$$

$$Q_6(1/2) = \frac{27}{16} - \frac{9}{8} e^{-1/2} - \frac{3}{8} e^{1/2} - \frac{113}{64} e^{-1} + \frac{45}{64} e$$

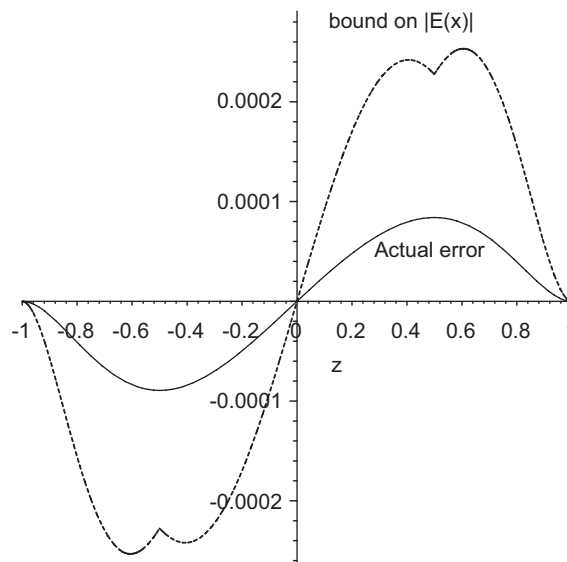


Fig. 1. Illustration of the maximum error bound with the second example.

and use these values in (9) to get $Q_6(x)$. To find the error bound in (23), we find $\|A^{-1}\|_\infty = \frac{3}{2}$ and use $|f^{(6)}(\bar{c})| = \max_{x \in [-1, 1]} |f^{(6)}(x)| = e$. We obtain

$$E(x) \leq \frac{|x(x^2 - 1)e|}{5040} \left[\left| x^2 - \frac{1}{4} \right| + \frac{3}{2} \left(\left| x - \frac{1}{2} \right| + \left| x + \frac{1}{2} \right| \right) \right].$$

Fig. 1 shows the actual error in the second example compared to the error bound given by (23). Where the actual error is negative, we have shown a negative error bound.

5. Uniqueness for special cases

The structure of the matrix A given by (14) and (15) allows us to determine whether a unique solution exists for certain sets of knots. We have a unique solution if and only if A is non-singular. Note that whether the matrix (14) is singular is not affected by the transformations, $\hat{s}_i = \alpha s_i + \beta$, $\hat{x}_i = \alpha x_i + \beta$ and $\hat{t}_i = \alpha t_i + \beta$, since we have

$$\frac{1}{\hat{x}_i - \hat{s}_j} = \frac{1}{\alpha(x_i - s_j)}, \quad \frac{1}{\hat{x}_i - \hat{x}_j} = \frac{1}{\alpha(x_i - x_j)} \quad \text{and} \quad \frac{1}{\hat{x}_i - \hat{t}_j} = \frac{1}{\alpha(x_i - t_j)}.$$

Hence $\det \hat{A} = \det A / \alpha^m$ where \hat{A} is formed using the \hat{t}_i, \hat{s}_i and \hat{x}_i and A is formed using the t_i, s_i and x_i . The following cases are examined:

Case 1: Take the case where there are only function values or first derivative values. Let the derivative knots be any subset of the zeroes of $\phi'(x)$ where $\phi(x)$ is the k th degree polynomial whose zeroes are the function knots ($\phi(x) = \prod_{r=1}^k (x - t_r)$). Here $m \leq k - 1$. We show the matrix A is singular.

Case 2: Again we take the case where there are only function values or first derivative values. Let the function knots be the set $\{-1, 1\} \cup \{z_i, 1 \leq i \leq v - 1\}$, where $z_i, 1 \leq i \leq v - 1$, are the zeroes of $P'_v(x)$, where $P_v(x)$ is the v th degree Legendre polynomial. Let the derivative knots be any subset of the zeroes of $P_v(x)$. Here $k = v + 1$. We show A is singular. This selection of knots could arise for example in obtaining higher order approximations after using collocation on two point boundary value problems (see [7]).

Case 3: Let the function knots be symmetric about a center point. Let the knots where both the function values and first derivative values are known be symmetric about the same point. Let the knots where only the first derivative values are known also be symmetric about the same center point and let the number of these knots be odd. We show A is singular. This selection of knots could arise for example in aspects for Runge–Kutta defect control (see [8]).

Case 4: Take the case where there are only function values or first derivative values. Let the function knots be the set $\{-1, 1\}$ or $\{-1, 0, 1\}$. Let the derivative knots be the zeroes of the m th degree Legendre polynomial. We show A is singular. The selection of $\{-1, 1\}$ for the function knots and zeroes of the m th degree Legendre polynomial, with m even, for the derivative values is discussed by Pruess and Jin in [16] and Jin and Pruess in [9] as a possible set of collocation points. They reject this set since it is singular.

For case 1, if we add rows 2, 3, \dots , m to row 1 in the determinant of A , given by (15) we obtain

$$\det A = \begin{vmatrix} \frac{\phi'(x_1)}{\phi(x_1)} & \frac{\phi'(x_2)}{\phi(x_2)} & \cdots & \frac{\phi'(x_m)}{\phi(x_m)} \\ \frac{1}{x_2 - x_1} & \frac{\phi'(x_2)}{\phi(x_2)} + \sum_{\substack{r=1 \\ r \neq 2}}^m \frac{1}{x_2 - x_r} & \cdots & \frac{1}{x_2 - x_m} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{1}{x_m - x_1} & \frac{1}{x_m - x_2} & \cdots & \frac{\phi'(x_m)}{\phi(x_m)} + \sum_{\substack{r=1 \\ r \neq m}}^m \frac{1}{x_m - x_r} \end{vmatrix}.$$

Since $\phi'(x_i) = 0$ for $i = 1, \dots, m$, therefore A is singular.

For case 2 we can write

$$\phi(x) = (x^2 - 1) \prod_{i=1}^{v-1} (x - z_i) = \frac{(x^2 - 1)P'_v(x)}{vp_v},$$

where p_v is the coefficient of x^v in $P_v(x)$. Using the identity

$$\left(\frac{(x^2 - 1)P'_v(x)}{v(v+1)} \right)' = P_v(x)$$

(see for example [11]), we obtain

$$\phi'(x) = \left(\frac{(x^2 - 1)P'_v(x)}{vp_v} \right)' = \frac{(v+1)}{p_v} P_v(x).$$

Hence case 2 is an example of case 1.

For case 3, since m is odd, we must have both k and l even. Let $k = 2u$, $l = 2w$ and $m = 2v + 1$. Let the points be symmetric about 0. We arrange all of the knots such that

$$\begin{aligned} t_{i+u} &= -t_i, \quad 1 \leq i \leq u, & s_{i+w} &= -s_i, \quad 1 \leq i \leq w, \\ x_{v+1} &= 0, & x_{i+v+1} &= -x_i, \quad 1 \leq i \leq v. \end{aligned} \quad (24)$$

Now write the matrix A in (14) as the block matrix

$$A = \begin{bmatrix} B & U & C \\ Y & G & Z \\ D & W & E \end{bmatrix},$$

where $B = [b_{ij}]$, $C = [c_{ij}]$, $D = [d_{ij}]$ and $E = [e_{ij}]$ are all $v \times v$ matrices, $U = [u_i]$ and $W = [w_i]$ are $v \times 1$ matrices, $Y = [y_j]$ and $Z = [z_j]$ are $1 \times v$ matrices and G is a single element. We form the new matrix \bar{A} , from A , whose determinant is the same as A , by adding column $r + v + 1$ to column r , and then adding row r to row $r + v + 1$, $1 \leq r \leq v$. We have

$$\bar{A} = \begin{bmatrix} \bar{B} & U & C \\ \bar{Y} & G & Z \\ \bar{D} & \bar{W} & \bar{E} \end{bmatrix},$$

where

$$\bar{B} = B + C, \quad \bar{Y} = Y + Z, \quad \bar{D} = B + C + D + E, \quad \bar{W} = W + U \quad \text{and} \quad \bar{E} = E + C. \quad (25)$$

From (14) and (24) we have

$$\begin{aligned}
 b_{ij} &= \begin{cases} 2 \sum_{r=1}^{2w} \frac{1}{x_i - s_r} + \sum_{r=1}^{2u} \frac{1}{x_i - t_r} + \sum_{\substack{r=1 \\ r \neq i}}^{2v+1} \frac{1}{x_i - x_r} & \text{if } i = j, \\ \frac{1}{x_i - x_j} & \text{if } i \neq j, \end{cases} \\
 &= \begin{cases} 2 \sum_{r=1}^w \left(\frac{1}{x_i - s_r} + \frac{1}{x_i + s_r} \right) + \sum_{r=1}^u \left(\frac{1}{x_i - t_r} + \frac{1}{x_i + t_r} \right) \\ \quad + \frac{3}{2x_i} + \sum_{\substack{r=1 \\ r \neq i}}^v \left(\frac{1}{x_i - x_r} + \frac{1}{x_i + x_r} \right) & \text{if } i = j, \\ \frac{1}{x_i - x_j} & \text{if } i \neq j, \end{cases} \\
 c_{ij} &= \begin{cases} \frac{1}{x_i - x_{i+v+1}} = \frac{1}{2x_i} & \text{if } i = j, \\ \frac{1}{x_i - x_{j+v+1}} = \frac{1}{x_i + x_j} & \text{if } i \neq j, \end{cases} \\
 d_{ij} &= \begin{cases} \frac{1}{x_{i+v+1} - x_i} = \frac{-1}{2x_i} & \text{if } i = j, \\ \frac{1}{x_{i+v+1} - x_j} = \frac{-1}{x_i + x_j} & \text{if } i \neq j, \end{cases} \\
 e_{ij} &= \begin{cases} 2 \sum_{r=1}^{2w} \frac{1}{x_{i+v+1} - s_r} + \sum_{r=1}^{2u} \frac{1}{x_{i+v+1} - t_r} + \sum_{\substack{r=1 \\ r \neq i+v+1}}^{2v+1} \frac{1}{x_{i+v+1} - x_r} & \text{if } i = j, \\ \frac{1}{x_{i+v+1} - x_{j+v+1}} & \text{if } i \neq j, \end{cases} \\
 &= \begin{cases} 2 \sum_{r=1}^w \left(\frac{-1}{x_i + s_r} + \frac{-1}{x_i - s_r} \right) + \sum_{r=1}^u \left(\frac{-1}{x_i + t_r} + \frac{-1}{x_i - t_r} \right) \\ \quad - \frac{3}{2x_i} + \sum_{\substack{r=1 \\ r \neq i}}^v \left(\frac{-1}{x_i + x_r} + \frac{-1}{x_i - x_r} \right) & \text{if } i = j, \\ \frac{-1}{x_i - x_j} & \text{if } i \neq j. \end{cases}
 \end{aligned}$$

We also have

$$u_i = \frac{1}{x_i}, \quad w_i = \frac{1}{x_{i+v+1}} = \frac{-1}{x_i}, \quad y_j = \frac{1}{x_j}, \quad z_j = \frac{1}{x_{j+v+1}} = \frac{-1}{x_j},$$

and

$$G = 2 \sum_{r=1}^{2w} \frac{1}{-s_r} + \sum_{r=1}^{2u} \frac{1}{-t_r} + \sum_{\substack{r=1 \\ r \neq v+1}}^{2v+1} \frac{1}{x_r} = 0.$$

From (24) we see that $\bar{D}=0$, $\bar{Y}=0$ and $\bar{W}=0$. Therefore \bar{A} is a $(2v+1) \times (2v+1)$ matrix with a lower $(v+1) \times (v+1)$ block all zero and therefore has determinant 0. Hence A is singular.

For case 4, if m is odd, we have an example of case 3 and the result follows. We concentrate on m even with $m = 2v$. Let

$$\eta(x_i) = \sum_{j=1}^k \frac{1}{x_i - t_j} = \begin{cases} \frac{2x_i}{x_i^2 - 1} & \text{if } \{t_1, t_2\} = \{-1, 1\}, \\ \frac{2x_i}{x_i^2 - 1} + \frac{1}{x_i} & \text{if } \{t_1, t_2, t_3\} = \{-1, 0, 1\}. \end{cases} \quad (26)$$

The matrix A in (15) can be written as the block matrix

$$A = \begin{bmatrix} B & C \\ D & E \end{bmatrix},$$

where $B = [b_{ij}]$, $C = [c_{ij}]$, $D = [d_{ij}]$ and $E = [e_{ij}]$ are all $v \times v$ matrices. Since the zeroes of P_{2v} , the $(2v)$ th degree Legendre polynomial, are symmetric about the origin, we let $x_r = -x_{r+v}$, $1 \leq r \leq v$. Hence the elements of B are given by

$$b_{ij} = \begin{cases} \eta(x_i) + \sum_{\substack{r=1 \\ r \neq i}}^{2v} \frac{1}{x_i - x_r} = \eta(x_i) + \frac{1}{2x_i} + \sum_{\substack{r=1 \\ r \neq i}}^v \frac{2x_i}{x_i^2 - x_r^2} & \text{if } i = j, \\ \frac{1}{x_i - x_j} & \text{if } i \neq j. \end{cases}$$

We also have

$$c_{ij} = \begin{cases} \frac{1}{x_i - x_{i+v}} = \frac{1}{2x_i} & \text{if } i = j, \\ \frac{1}{x_i - x_{j+v}} = \frac{1}{x_i + x_j} & \text{if } i \neq j, \end{cases}$$

$$d_{ij} = \begin{cases} \frac{1}{x_{i+v} - x_i} = \frac{-1}{2x_i} & \text{if } i = j, \\ \frac{1}{x_{i+v} - x_j} = \frac{-1}{x_i + x_j} & \text{if } i \neq j, \end{cases}$$

and

$$e_{ij} = \begin{cases} \eta(x_{i+v}) + \sum_{\substack{r=1 \\ r \neq i+v}}^{2v} \frac{1}{x_{i+v} - x_r} = -\eta(x_i) - \frac{1}{2x_i} + \sum_{\substack{r=1 \\ r \neq i}}^v \frac{-2x_i}{x_i^2 - x_r^2} & \text{if } i = j, \\ \frac{1}{x_{i+v} - x_{j+v}} = \frac{-1}{x_i - x_j} & \text{if } i \neq j. \end{cases}$$

Now form the matrix \bar{A} whose elements are obtained from A by adding column $r + v$ to column r and row r to row $r + v$, $1 \leq r \leq v$. We have

$$\bar{A} = \begin{bmatrix} \bar{B} & \bar{C} \\ \bar{D} & \bar{E} \end{bmatrix},$$

where $\bar{B} = [\bar{b}_{ij}]$, $\bar{D} = [\bar{d}_{ij}]$ and $\bar{E} = [\bar{e}_{ij}]$ are all $v \times v$ matrices with $\bar{B} = B + C$, $\bar{D} = B + C + D + E$ and $\bar{E} = E + C$. We have $\det \bar{A} = \det A$. Note that $\bar{D} = 0$. Hence $\det \bar{A} = 0$ if $\det \bar{B} = 0$ or $\det \bar{E} = 0$. Using (26) we have

$$\bar{b}_{ij} = \begin{cases} \frac{2x_i}{x_i^2 - 1} + \frac{2x_i}{2x_i^2} + \sum_{\substack{r=1 \\ r \neq i}}^v \frac{2x_i}{x_i^2 - x_r^2} & \text{if } \{t_r\} = \{-1, 1\} \text{ and } i = j, \\ \frac{2x_i}{x_i^2 - x_j^2} & \text{if } i \neq j, \end{cases}$$

and

$$\bar{e}_{ij} = \begin{cases} -\frac{2x_j}{x_j^2 - 1} - \frac{2x_j}{2x_j^2} - \sum_{\substack{r=1 \\ r \neq j}}^v \frac{2x_j}{x_j^2 - x_r^2} & \text{if } \{t_r\} = \{-1, 0, 1\} \text{ and } i = j, \\ -\frac{2x_j}{x_i^2 - x_j^2} & \text{if } i \neq j. \end{cases}$$

Therefore either \bar{B} or \bar{E} is singular if the matrix W whose elements are given by

$$w_{ij} = \begin{cases} \frac{1}{x_i^2 - 1} + \frac{1}{2x_i^2} + \sum_{\substack{r=1 \\ r \neq i}}^v \frac{1}{x_i^2 - x_r^2} & \text{if } i = j, \\ \frac{1}{x_i^2 - x_j^2} & \text{if } i \neq j \end{cases}$$

is singular. But the rows of W add to 0 since

$$\begin{aligned} \sum_{j=1}^v w_{ij} &= \frac{1}{x_i^2 - 1} + \frac{1}{2x_i^2} + 2 \sum_{\substack{r=1 \\ r \neq i}}^v \frac{1}{x_i^2 - x_r^2} \\ &= \frac{1}{x_i^2 - 1} + \frac{P''_{2v}(x_i)}{2x_i P'_{2v}(x_i)} \\ &= 0. \end{aligned}$$

Here we have used the fact that since m is even we can write the m th degree Legendre polynomial as $P_{2v} = \prod_{r=1}^v (x^2 - x_r^2)$ and therefore

$$\frac{P''_{2v}(x_i)}{2x_i P'_{2v}(x_i)} = \frac{1}{2x_i^2} + 2 \sum_{\substack{r=1 \\ r \neq i}}^v \frac{1}{x_i^2 - x_r^2}.$$

In addition, we have used the property of Legendre polynomials that

$$[(1 - x^2)P'_{2v}(x)]' = 2v(2v + 1)P_{2v}(x).$$

This completes case 4.

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