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Polynomial Algebra for Birkhoff Interpolants

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Abstract We introduce a unifying formulation of a number of related problems which can all be solved using a contour integral formula. Each of these problems requires finding a non-trivial linear combination of some of the values of a function f, and its first and higher derivatives, at a number of data points. This linear combination is required to have zero value when f is a polynomial of up to a specific degree p. Examples of this type of problem include Lagrange, Hermite and Hermite-Birkhoff interpolation; and various numerical quadrature and differentiation formulae. Other applications include the estimation of missing data and root-finding.

Keywords Lagrange, Hermite, and Hermite-Birkhoff interpolation · Contour integrals · Barycentric form · Root-finding

Mathematics Subject Classification (2000) 41A05 · 65D05 · 65D25 · 65D30

1 Introduction

The purpose of this paper is to present a number of approximation formulae using a single standard formulation. These include formulae for Lagrange, Hermite and Hermite–Birkhoff interpolation, divided difference formulae, numerical quadrature and numerical differentiation. Each of these approximation formulae can be written as a non-trivial linear combination

$$\sum_{i=1}^{n} \sum_{j \in S_i} \widehat{a}_{ij} f^{(j)}(\tau_i) = 0, \tag{1}$$

where f is a polynomial of degree not exceeding p, and S_i is a subset of $\{0, 1, \ldots, s_i - 1\}$ such that $s_i - 1 \in S_i$. The value of p is $-2 + \sum_{i=1}^{n} |S_i|$, where $|S_i|$ is the cardinality of S_i.

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If $S_i = \{0, 1, \ldots, s_i - 1\}$, for each $i = 1, 2, \ldots, n$, we will rewrite (1) in the form

$$\sum_{i=1}^{n} \sum_{j=0}^{s_i-1} a_{ij} f^{(j)}(\tau_i) = 0. \tag{2}$$

The common feature of these formulations is their relation to contour integrals of the form

$$\frac{1}{2\pi i} \oint_C R(z) f(z) dz, \tag{3}$$

where R is a rational function related to the problem. By using the Cauchy integral formula we will find the approximation we require.

The paper is organized as follows: a review of known literature on Hermite–Birkhoff interpolation and related problems will be presented in Section 2. This is followed by Section 3, where the central result is given and by Section 4 where diverse applications are considered. Results and discussion on the existence and other properties of these approximations are presented in Section 5.

2 Literature review

3 Solution by contour integrals

3.1 Statement of the problem

We are concerned with a function f and various approximations related to it. The approximations will have order p, in the sense that if f is replaced by a polynomial of degree p, then the approximation will be exact. The approximations will all have the form

$$\sum_{i=1}^{n} \sum_{j=0}^{s_i-1} a_{ij} f^{(j)}(\tau_i) = 0, \quad \deg(f) \le p. \tag{4}$$

Because of its relation to Hermite interpolation, we will refer to the construction of approximations satisfying (4) as the "Hermite case". In Subsection 3.2 we will obtain formulae for the coefficients a_{ij}.

A more general problem, which we will refer to as the "Birkhoff case", is to assume that there is missing data. In other words, we will assume that for each i, $f^{(j)}(\tau_i)$ is given only for a subset S_i of $\{0, 1, \ldots, s_i - 1\}$. We will assume that such a subset always contains $s_i - 1$. As a matter of parsimony, this will enable us to avoid the situation that s_i could have been replaced by a lower integer.[1] With this more general case, (4) will be replaced by

$$\sum_{i=1}^{n} \sum_{j \in S_i} \widehat{a}_{ij} f^{(j)}(\tau_i) = 0, \quad \deg(f) \le p. \tag{5}$$

[1] Our MAPLE and MATLAB codes make no such restriction, though—they simply do more work than strictly necessary and give an answer equivalent to the most parsimonious approach, although containing extra factors in numerator and denominator that cancel out.

By counting the number of constraints, we would hope to be able to solve (4) with $p = -2 + \sum_{i=1}^{n} s_i$. In the Birkhoff case, again by counting constraints, we see that it is appropriate to aim for an order

$$p = -2 + \sum_{i=1}^{n} |S_i|. \tag{6}$$

Conditions under which (5) is guaranteed to have a solution will be discussed in Section 5.

3.2 Solution using contour integrals in the Hermite case

Given an approximation problem in the Hermite case, we define $w(z)$ by

$$w(z) = \prod_{i=1}^{n} (z - \tau_i)^{s_i}, \tag{7}$$

where the τ_i and s_i are as in (4). We have the following lemma.

Lemma 1 *Let f be a polynomial of degree not exceeding $p = -2 + \sum_{i=1}^{n} s_i$, then*

$$\frac{1}{2\pi i} \oint_C \frac{f(z)}{w(z)} dz = 0, \tag{8}$$

where $w(z)$ is defined by (7) *and the contour C is a circle with centre* 0 *and radius R greater than* $\max_{i=1}^{n} |\tau_i|$.

Proof The proof is a classic result in Complex Analysis and can be found in [5, Thm. 8.1, p. 233]. □

We can now write $w(z)^{-1}$ in (8) in partial fractions

$$\frac{1}{w(z)} = \sum_{i=1}^{n} \sum_{j=0}^{s_i - 1} \frac{\gamma_{ij}}{(z - \tau_i)^{j+1}}, \tag{9}$$

so that substituting (9) into (8) and evaluating term by term, we find the result

$$\sum_{i=1}^{n} \sum_{j=0}^{s_i - 1} \frac{\gamma_{ij}}{j!} f^{(j)}(\tau_i) = 0. \tag{10}$$

Hence, we can solve (4) using

$$a_{ij} = \frac{\gamma_{ij}}{j!}. \tag{11}$$

To evaluate the a_{ij} in a convenient form, we use the following result, which is equivalent to the local series method for computing the partial fraction expansion of $1/w(z)$. Many sources contain this algorithm, for example [4, v. 1, p. 555]. Faster algorithms are known, see e.g. [7], but they can be significantly less stable numerically. We include a description of the algorithm here, for convenience; our Matlab and Maple implementations of this algorithm use the recurrence relation (13) below.

Lemma 2 *Let K denote a finite set of integers, and define $\chi_1, \chi_2, \ldots$ by the formula*

$$\chi_0 + \chi_1 t + \chi_2 t^2 + \ldots = \chi_0 \prod_{k \in K} (1 - t\theta_k)^{-s_k} \,, \tag{12}$$

where χ_0 is given. Then, $\chi_1, \chi_2, \ldots$ satisfy the recurrence relation

$$\chi_j = \frac{1}{j} \sum_{\ell=0}^{j-1} \chi_\ell \phi_{j-\ell} \,, \tag{13}$$

where $\phi_j = \sum_{k \in K} s_k \theta_k^j$.

Proof From the logarithmic series we have

$$\ln(1 - \theta_k t) = -\sum_{j=1}^{\infty} \frac{t^j}{j} \theta_k^j \,, . \tag{14}$$

For $|t|$ sufficiently small, it follows by multiplying by $-s_k$ and summing over $k \in K$, that

$$\ln\Big(\prod_{k \in K} (1 - t\theta_k)^{-s_k} \Big) = \sum_{j=1}^{\infty} \frac{t^j}{j} \phi_j \,, \tag{15}$$

and therefore

$$\chi_0 + \chi_1 t + \chi_2 t^2 + \cdots = \chi_0 \exp\left(\sum_{j=1}^{\infty} \frac{t^j}{j} \phi_j \right) . \tag{16}$$

Differentiate (16) with respect to t and it follows that

$$\chi_1 t + 2\chi_2 t + 3\chi_3 t^2 + \cdots = (\phi_1 + \phi_2 t + \cdots)(\chi_0 + \chi_1 t + \chi_2 t^2 + \cdots) \,. \tag{17}$$

Equate the coefficients of t^{j-1} and (13) follows. □

In our application of this lemma, let

$$K = \{1, 2, \ldots, n\} \setminus \{i\}, \quad \theta_k = \frac{1}{\tau_k - \tau_i}, \quad \chi_0 = \prod_{k \in K} (\tau_i - \tau_k)^{-s_k}, \quad t = z - \tau_i.$$

For a given $i \in \{1, 2, \ldots, n\}$, evaluate the Laurent expansion about $z = \tau_i$ as follows

$$\begin{aligned} \frac{1}{w(z)} &= \frac{1}{(z - \tau_i)^{s_i}} \prod_{k \in K} (z - \tau_k)^{-s_k} \\ &= \frac{1}{(z - \tau_i)^{s_i}} \prod_{k \in K} \Big((\tau_i - \tau_k) \Big(1 - \frac{z - \tau_i}{\tau_k - \tau_i} \Big) \Big)^{-s_k} \\ &= \frac{1}{(z - \tau_i)^{s_i}} \chi_0 \prod_{k \in K} (1 - t\theta_k)^{-s_k} \\ &= \frac{1}{(z - \tau_i)^{s_i}} (\chi_0 + \chi_1 (z - \tau_i) + \chi_2 (z - \tau_i)^2 + \cdots) \end{aligned} \tag{18}$$

and hence

$$\gamma_{ij} = \chi_{s_i - j - 1}, \quad a_{ij} = \frac{\chi_{s_i - j - 1}}{j!}. \tag{19}$$

Having found the coefficients in (4), we generalize to the Birkhoff case.

3.3 Solution in the Birkhoff case

To allow for missing data, replace (8) by

$$\frac{1}{2\pi i}\oint_C \frac{B(z)f(z)}{w(z)}dz = 0, \tag{20}$$

where

$$B(z) = b_0 + b_1 z + \cdots + b_m z^m \tag{21}$$

and m is the number of missing data items. The integral is still zero if f is now restricted to a polynomial of degree

$$p = -2 - m + \sum_{i=1}^{n} s_i = -2 + \sum_{i=1}^{n} |S_i|. \tag{22}$$

The coefficients in $B(z)$, suitably normalized, are to be chosen so that, in the partial fraction expansion of $B(z)/w(z)$, which we will write as

$$\frac{B(z)}{w(z)} = \sum_{i=1}^{n}\sum_{j=0}^{s_i-1} \frac{\widehat{\gamma}_{ij}}{(z-\tau_i)^{j+1}}, \tag{23}$$

the value of $\widehat{\gamma}_{ij}$ will vanish whenever $j \notin S_i$. To solve (5), it is then possible to use a slightly modified form of Lemma 1 to give the result

$$\widehat{a}_{ij} = \frac{\widehat{\gamma}_{ij}}{j!}, \quad j \in S_i. \tag{24}$$

We compute the coefficients $\widehat{\gamma}_{ij}$ by multiplying the local series for $B(z)$ with the partial fraction decomposition of $1/w(z)$. The coefficients are computed with Cauchy convolution, which we write in matrix notation in the Theorem below.

Theorem 1 *For $i = 1, 2, \ldots, n$, let $\mathbf{M}_i$ denote the $s_i \times (m+1)$ matrix*

$$\mathbf{M}_i = \mathbf{\Gamma}_i \mathbf{T}_i, \tag{25}$$

where $\mathbf{\Gamma}_i$ is the $s_i \times s_i$ matrix

$$\mathbf{\Gamma}_i = \begin{bmatrix} \gamma_{i,0} & \gamma_{i,1} & \cdots & \gamma_{i,s_i-2} & \gamma_{i,s_i-1} \\ \gamma_{i,1} & \gamma_{i,2} & \cdots & \gamma_{i,s_i-1} & 0 \\ \vdots & & & & \vdots \\ \gamma_{i,s_i-1} & 0 & \ldots & 0 & 0 \end{bmatrix}, \tag{26}$$

where for $0 \leqslant j \leqslant s_i - 1$ and $0 \leqslant k \leqslant s_i - 1$, the (j,k) entry (indexing from 0) of $\mathbf{\Gamma}_i$ is

$$\mathbf{\Gamma}_i(j,k) = \begin{cases} \gamma_{i,k+j} & \text{if } k+j \leqslant s_i - 1 \\ 0 & \text{otherwise} \end{cases} \tag{27}$$

and $\mathbf{T}_i$ is the $s_i \times (m+1)$ matrix

$$\mathbf{T}_i = \begin{bmatrix} 1 & \tau_i & \tau_i^2 & \ldots & \tau_i^m \\ & 1 & 2\tau_i & \ldots & m\tau_i^{m-1} \\ & & 1 & \ldots & \frac{m(m-1)}{2!}\tau_i^{m-2} \\ & & & \ddots & \vdots \end{bmatrix}, \tag{28}$$

with the (j,k) element

$$\mathbf{T}_i(j,k) = \binom{k}{j} t_i^{k-j} , \tag{29}$$

and the last row allows computation of the (s_i-1)*th derivative of* B *evaluated at* τ_i. *[Recall that* $\binom{k}{j}=0$, *if* $j>k$.*] Let* $\widetilde{\mathbf{M}}$ *denote the* $m\times(m+1)$ *matrix*

$$\widetilde{\mathbf{M}} = \begin{bmatrix} \widetilde{M}_1 \\ \widetilde{M}_2 \\ \vdots \\ \widetilde{M}_n \end{bmatrix} , \tag{30}$$

where $\widetilde{M}_i$ *consists of rows of* $\mathbf{M}_i$ *such that row number* j *is included if and only if* $j \notin S_i$.

Then, if $\widetilde{\mathbf{M}}$ *has rank* m, *the coefficients in* (21) *are a non-zero solution of*

$$\widetilde{\mathbf{M}}\mathbf{b} = 0 , \quad \textit{where} \quad \mathbf{b} = \begin{bmatrix} b_0 \; b_1 \; \ldots \; b_m \end{bmatrix}^T . \tag{31}$$

Proof The proof requires finding m homogeneous linear equations in the elements of $\mathbf{b}$. This, in turn, requires finding the values of $\widetilde{\gamma}_{ij}$ in (24), in terms of $\mathbf{b}$. The first step is to write the Taylor coefficients about τ_i in terms of $\mathbf{b}$. This is given by the formula

$$\begin{bmatrix} B(\tau_i) \\ B'(\tau_i) \\ \frac{1}{2!}B''(\tau_i) \\ \vdots \\ \frac{1}{(s_i-1)!}B^{(s_i-1)}(\tau_i) \end{bmatrix} = \mathbf{T}_i \mathbf{b}. \tag{32}$$

The values of $\widehat{\gamma}_{ij}$, for $j=0,1,\ldots,s_i-1$, are found by multiplying (9) by

$$B(z) = B(\tau_i) + B'(\tau_i)(z-\tau_i) + \cdots + \frac{1}{(s_i-1)!}B^{(s_i-1)}(\tau_i)(z-\tau_i)^{s_i-1} + O((z-\tau_i)^{s_i}). \tag{33}$$

[Note that some of those derivatives will be zero if $s_i > m$.] This gives

$$\widehat{\gamma}_{ij} = \sum_{\ell=0}^{\min(j,m)} \gamma_{i\ell} \frac{B^{(\ell)}(\tau_i)}{\ell!}, \tag{34}$$

which can be written as

$$\begin{bmatrix} \widehat{\gamma}_{i0} \\ \widehat{\gamma}_{i1} \\ \vdots \\ \widehat{\gamma}_{i,s_i-1} \end{bmatrix} = \mathbf{\Gamma}_i \begin{bmatrix} B(\tau_i) \\ B'(\tau_i) \\ \frac{1}{2!}B''(\tau_i) \\ \vdots \\ \frac{1}{(s_i-1)!}B^{(s_i-1)}(\tau_i) \end{bmatrix} . \tag{35}$$

Substitute from (32) and use (25); we find that

$$\begin{bmatrix} \widehat{\gamma}_{i0} \\ \widehat{\gamma}_{i1} \\ \vdots \\ \widehat{\gamma}_{i,s_i-1} \end{bmatrix} = \mathbf{\Gamma}_i(\mathbf{T}_i\mathbf{b}) = \mathbf{M}_i\mathbf{b} \tag{36}$$

and because $\widehat{\gamma}_{ij} = 0$ for $j \notin S_i$, it follows that $\widetilde{\mathbf{M}_i}\mathbf{b} = 0$. Combine this result for all $i = 1, 2, \ldots, n$ and the theorem follows. □

As in Subsection 3.2. we conclude this investigation of the Birkhoff case by finding the coefficients in(5). These are

$$\widehat{a}_{ij} = \frac{\widehat{\gamma}_{ij}}{j!}, \qquad i \in \{1, 2, \ldots, n\}, j \in S_i. \tag{37}$$

4 Specific applications

4.1 Interpolation

Given data points as in Section 3, we can obtain a formula for the interpolating polynomial by adding to the set $\{\tau_1, \tau_2, \ldots, \tau_n\}$ the additional point $\tau_0 = t$, with $s_0 = 1$. This means, in the Hermite case, that we make use of the contour integral (8) in which $w(z)$ is replaced by

$$w(z) = \prod_{i=0}^{n} (z - \tau_i)^{s_i} = (z - t) \prod_{i=1}^{n} (z - \tau_i)^{s_i} \tag{38}$$

Following through with the construction of Subsection 3.2, we find the modified form of (4) as follows:

$$a_{00}(t) f(t) + \sum_{i=1}^{n} \sum_{j=0}^{s_i-1} a_{ij}(t) f^{(j)}(\tau_i) = 0, \quad \deg(f) \le -1 + \sum_{i=1}^{n} s_i. \tag{39}$$

Assuming that $a_{00}(t) \neq 0$, this gives the interpolation formula

$$f(t) = \sum_{i=1}^{n} \sum_{j=0}^{s_i-1} \frac{-a_{ij}(t)}{a_{00}(t)} f^{(j)}(\tau_i), \quad \deg(f) \le -1 + \sum_{i=1}^{n} s_i. \tag{40}$$

A priori it is not clear that the expression for $f(t)$ is polynomial in t; we shall discuss later just why it is indeed polynomial. In the Birkhoff case, we can do the construction described in Subsection 3.3, again with $w(z)$ replaced by (38). This gives a formula

$$f(t) = \sum_{i=1}^{n} \sum_{j \in S_i} \frac{-\widehat{a}_{ij}(t)}{\widehat{a}_{00}(t)} f^{(j)}(\tau_i), \quad \deg(f) \le -1 + \sum_{i=1}^{n} |S_i|, \tag{41}$$

again assuming that $\widehat{a}_{00}(t) \neq 0$. Again this is polynomial in t.

If we have a particular numerical value of t, or only a few such values, for which we need to evaluate $f(t)$, then perhaps it makes sense to construct these coefficients $\widehat{a}_{00}(t)$

and $\widehat{a}_{ij}(t)$ anew for each t. If, however, we have a great many values of t for which we need to evaluate f, then perhaps it makes sense to do the construction "once and for all". This is indeed possible. The linear system defining the unknown coefficients of $B(z)$ then contains a matrix and right-hand-side that depend polynomially on the symbol t. Solving this system is then a *symbolic computation*, and therefore more expensive, but still feasible in many applications. An alternative approach that may be cheaper, filling in missing data, is discussed in Section 4.2.

Example 1 Let $\tau = [0, r, 1]$ with data given as $f(0)$, $f'(r)$, and $f(1)$. We do not yet specify r, but for the moment imagine it is a real number between 0 and 1. Finding a polynomial of degree 2 that fits this data is a Hermite-Birkhoff problem. We begin by defining $w(z) = z(z-r)^2(z-1)$, adding a new node $\tau_0 = t$ and making all necessary changes in our notation to make this example clear, and computing the partial fraction decomposition of

$$\begin{aligned}\frac{1}{(z-t)w(z)} = {} & \frac{1}{r\,(-1+r)\,(-t+r)\,(z-r)^2} - \frac{1}{(-1+r)^2\,(t-1)\,(z-1)} \\ & + \frac{1}{t\,(-t+r)^2\,(t-1)\,(z-t)} + \frac{1}{r^2 tz} \\ & + \frac{-t+2\,r+2\,rt-3\,r^2}{(z-r)\,r^2\,(-1+r)^2\,(-t+r)^2}\,.\end{aligned} \tag{42}$$

The matrices of Theorem 1 that we need are, therefore, simple: $\widetilde{M}_0$ is empty, as is $\widetilde{M}_1$ and $\widetilde{M}_3$, but we must have one row present in $\widetilde{M}_2$, namely

$$\widehat{\gamma}_{2,0}(b_0(t) + b_1(t)r) + \widehat{\gamma}_{2,1}b_1(t) = 0\,. \tag{43}$$

Enforcing this will ensure that the residue multiplying the unknown value of f at r will be zero. Clearly, we have one constraint and two unknowns b_0 and b_1, each of which depend on t; it is convenient to add a normalization condition, namely that the residue at $z = t$, our new symbolic node, is -1. This will allow easy isolation of the value of $f(t)$ from the resulting zero sum of residues. This residue is

$$\frac{b_0(t) + b_1(t)t}{w(t)} = -1\,. \tag{44}$$

The determinant of the 2×2 matrix of these equations (43,44) is

$$\mathrm{Det} = \frac{2r-1}{r^2(1-r)^2}\,, \tag{45}$$

which clearly identifies the problematic cases $r = 0$ and $r = 1$ when our formulation is structurally discontinuous, and the case $r = 1/2$ when the problem is not poised.

If r is not 0, 1/2, or 1, the system can be solved for the unknowns and the resulting residues computed, giving the barycentric formula

$$f(t) = w\,(t)\left(\frac{(t+1-2\,r)\,f\,(0)}{t\,(2\,r-1)\,(t-r)^2} + \frac{f'\,(r)}{(2\,r-1)\,(t-r)^2} + \frac{(2\,r-t)\,f\,(1)}{(t-r)^2\,(2\,r-1)\,(t-1)}\right) \tag{46}$$

Notice that $w(t) = t(t-r)^2(t-1)$ contains a factor that exactly cancels each of the t, $t-1$, and $(t-r)^2$ factors in each term of the barycentric formula. The end result is a polynomial in t. One could, if one wanted, rewrite the polynomial and express it in the monomial basis. We stress that doing so is, in general, a bad idea.

Remark 1 When we are missing m pieces of data, we need only solve an m by m linear system, symbolic in that it contains the symbol t; here we solved an $m+1$ by $m+1$ system (symbolic both in t and in the parameter r) because we chose to normalize by making the residue at $z=t$ to be -1, instead of taking $B(z)$ to be monic, $B(z) = b_0(t) + z$. This is a matter of taste, which makes no practical difference in the method.

4.2 Filling in missing data

We discuss the problem of inserting some or all of the data which was not originally available in an instance of the Birkhoff case. The inserted data is to be calculated from the interpolating polynomial defined by the original Hermite-Birkhoff data, which we assume is poised. However, this problem can also be looked at in terms of the zero-valued linear combination of the original data and a single additional piece of data, which is to hold for all polynomials of up to degree $-1 + \sum_{i=1}^{n} |S_i|$. We illustrate the process by an example, but note that the process has been implemented in a general MATLAB program, written by Piers Lawrence at our request.

Example 2 Suppose that $\tau = [1, 2, 4]$, (this is equivalent to the previous example, with a linear change of variable and specifying $r = 1/3$) and that we know $f(1)$, $f'(2)$, and $f(4)$. We will use the residue method to find $f(2)$. Here, $w(z) = (z-1)(z-2)^2(z-4)$. Unlike the case where we wish to find f at an arbitrary point $z = t$, where we needed a degree $m = 1$ multiplier $B(z)$, here it suffices to take $B(z) = 1$. In general, we may use a degree $m-1$ multiplier. To continue, $w(z)^{-1}$ has the partial fraction expansion

$$\frac{1}{(z-1)(z-2)^2(z-4)} = -\frac{1/3}{z-1} + \frac{1/4}{z-2} - \frac{1/2}{(z-2)^2} + \frac{1/12}{z-4} \,. \tag{47}$$

For f a polynomial of degree not exceeding 2 we now have

$$0 = \frac{1}{2\pi i} \oint_C \frac{f(z)dz}{w(z)} = -\frac{1}{3}f(1) + \frac{1}{4}f(2) - \frac{1}{2}f'(2) + \frac{1}{12}f(4) \tag{48}$$

which immediately gives

$$f(2) = \tfrac{4}{3}f(1) + 2f'(2) - \tfrac{1}{3}f(4) \,. \tag{49}$$

Of course, this particular problem could have been solved by other approaches as well, for example by divided differences [6].

The general approach is to add a single pair (I, J) to the set of known data. That is, we suppose we wish to identify $f^{(J)}(\tau_I)$, which is not given by any (i, j) in $1 \le i \le n$, $j \in S_i$ (but τ_I is one of the interpolating nodes, and so we cannot use the approach of the previous section, which required that $t \ne \tau_i$ for each i). Now carry out the construction in Subsection 3.3, but here we do not set to zero the row corresponding to the pair (I, J); this gives us only the remaining $m-1$ conditions to satisfy. Thus, we need a multiplier $B(z)$ of only degree $m-1$. For convenience, as in example 1, we may use a degree m multiplier and set the residue for (I, J) to be -1, if this is possible. The resulting sum of residues is (in general)

$$a_{IJ} f^{(J)}(\tau_I) + \sum_{i=1}^{n} \sum_{j \in S_i} a_{ij} f^{(j)}(\tau_i) = 0 \tag{50}$$

Table 1 Relative error in a degree 23 Hermite-Birkhoff problem, solved in MATLAB by the fill-in method.

```
tau  = cos( (0:n)*pi/n ); % nodes
t    = linspace( -1, 1, 20*n+1 );
f = @(x) sin(pi*x);
df = @(x) pi*cos(pi*x);
ddf = @(x) -pi^2*sin(pi*x);
rho  = [f(tau); df(tau); ddf(tau)]; % data
rho(1,6)=NaN;
rho(1,7) = NaN;
rho(2,8)=NaN;
r    = rho(:);
r = birkhoff_interp1(r,tau,3)';
[w,D]   = genbarywts( tau, 3 ); % get barycentric weights
[y,yp]  = hermiteval( r, t, tau, 3, w, D ); % evaluate interpolant
```

If $a_{IJ} \neq 0$, this will allow us to identify the (formerly) missing piece of data. The connection between the interpolating polynomial and the fill-in result given by (50) is as follows.

Theorem 2 *If a_{IJ} in* (50) *is not zero, and $\varphi(t)$ is the unique interpolating polynomial determined by the poised Hermite-Birkhoff problem $f^{(j)}(\tau_i)$, $j \in S_i$, $i \in \{1, 2, \ldots, n\}$, then*

$$f^{(J)}(\tau_I) = \varphi^{(J)}(\tau_I). \tag{51}$$

Proof Since $\varphi(t)$ is a polynomial of degree not exceeding $-1 + \sum_{i=1}^{n} |S_i|$, (50) holds with f replaced by φ. That is,

$$a_{IJ}\varphi^{(J)}(\tau_I) + \sum_{i=1}^{n} \sum_{j \in S_i} a_{ij}\varphi^{(j)}(\tau_i) = 0. \tag{52}$$

Because of the interpolating property of φ, $\varphi^{(j)}(\tau_i) = f^{(j)}(\tau_i)$ for all $j \in S_i$, $i \in \{1, 2, \ldots, n\}$. Hence,

$$a_{IJ}\varphi^{(J)}(\tau_I) + \sum_{i=1}^{n} \sum_{j \in S_i} a_{ij} f^{(j)}(\tau_i) = 0. \tag{53}$$

Subtract (53) from (50), and the result follows. □

Example 3 In Table 1 we see some MATLAB statements defining a degree 23 (27 − 1 minus $m = 3$ missing data) Hermite-Birkhoff interpolation problem, together with calls to MATLAB routines that we have written to solve such problems. In Figure 1 we see a plot of the relative error of the polynomial *evaluated as a barycentric Hermite polynomial using the recovered (filled-in) data*. When the number of missing data is small, it is convenient as well as efficient to proceed in this manner. The MATLAB code `birkhoff_interp1` is available on request, and the other codes are available at `http://www.orcca.on.ca/ TechReports/ 2007/ TR-07-05.html`.

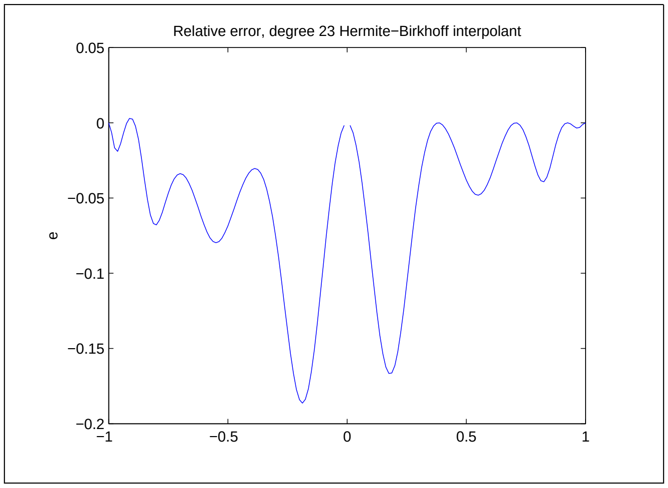

Fig. 1 Relative error $y/\sin(\pi t) - 1$ in a degree 23 Hermite-Birkhoff approximation (missing two function values and one derivative value).

4.3 Numerical quadrature and differentiation

4.4 Root-finding

We may wish to compute the roots of a univariate polynomial that is specified by a Hermite-Birkhoff interpolation problem. There are strong numerical and structural advantages in working with the given data directly without completing the interpolation and converting to the familiar monomial basis [3]. Numerically stable sets of basis-preserving root-finding algorithms, in the Hermite and Lagrange cases, have been used in [2].

In a similar fashion, if we have a Hermite-Birkhoff interpolation problem, we do not wish to first compute a monomial basis representation for the solution before finding the desired roots. Instead, we suggest that the approach of Section 4.2 be used to first fill in the missing data. Having done this, without completing the interpolation, we have converted the original problem to the Hermite case. We can then use existing algorithms to compute all roots of the given polynomial by solving a generalized eigenvalue problem. This is done by constructing a pair of regular matrices, known as the companion pencil matrices. The finite generalized eigenvalues of this matrix pencil are the roots of the original polynomial. We demonstrate this process with an example.

Example 4 As in example 2, let $\tau = [1, 2, 4]$. Suppose also that $f(1) = 1$, $f'(2) = 0$, and $f(4) = -1$. The 'fill-in' process gives

$$f(2) = \tfrac{4}{3} f(1) + 2f'(2) - \tfrac{1}{3} f(4) = \tfrac{5}{3} \,. \qquad (54)$$

The generalized companion matrix pencil of [2] is

$$C_0 = \begin{bmatrix} 1 & & & & 1 \\ & 2 & & & \frac{5}{3} \\ & 1 & 2 & & 0 \\ & & & 4 & -1 \\ \frac{1}{3} & -\frac{1}{4} & \frac{1}{2} & -\frac{1}{12} & 0 \end{bmatrix} \tag{55}$$

and C_1 is, as usual, the 5×5 identity matrix with the $(5, 5)$ corner being replaced by zero. Note that the generalized barycentric weights γ_{ij} appear in the bottom row, and the polynomial values appear in the final column. The nodes appear in transposed Jordan blocks along the diagonal. It is easy to see that $\det(tC_1 - C0) = f(t)$ for any t. We find the generalized eigenvalues numerically. There are three infinite eigenvalues (because f is degree 2 while the matrices are 5 by 5), and two finite eigenvalues: Maple's call to LAPACK routines gets 3.58113883008418021 and 0.418861169915851983. [The exact values are $2 \pm \sqrt{10}/2$.]

We remark that the roots were found *without* converting to a monomial basis at any time.

4.5 Rational interpolation

The approach described in this paper can be generalized to the rational polynomial case, with fixed denominator. This is interesting and useful because, as in [2], one can choose the denominator with parameters that can be *tuned* to ensure monotonicity, convexity, or other properties, as in [1]. In what follows, we assume $R(z) = f(z)/q(z)$ is the rational polynomial with $q(z)$ fixed and not identically zero.

Lemma 3 *Let $w(z)$ be defined as in (7). Suppose $\deg q(z) \leqslant -1 + \sum_{i=1}^{n} s_i$. Put $\sigma_{ij} = \frac{q^{(j)}(\tau_i)}{j!}$ for brevity. Then*

$$\frac{q(z)}{w(z)} = \sum_{i=1}^{n} \sum_{j=0}^{s_i-1} \frac{\alpha_{ij}}{(z-\tau_i)^{j+1}} \tag{56}$$

where

$$\alpha_{ij} = \sum_{k=0}^{s_i-1-j} \gamma_{i,j+k}\sigma_{ik}\,. \tag{57}$$

Moreover, if $q(\tau_i) \neq 0$, and γ_{i,s_i-1} is as defined in (19) then

$$\alpha_{i,s_i-1} = \gamma_{i,s_i-1}\sigma_{i,0} \neq 0. \tag{58}$$

Proof By the Hermite interpolation formula,

$$\frac{q(z)}{w(z)} = \sum_{i=1}^{n} \sum_{j=0}^{s_i-1} \sum_{k=0}^{j} \gamma_{ij}\sigma_{ik}(z-\tau_i)^{k-j-1} \tag{59}$$

Interchanging the order of the second and third sums,

$$\frac{q(z)}{w(z)} = \sum_{i=1}^{n} \sum_{k=0}^{s_i-1} \sum_{j=k}^{s_i-1} \gamma_{ij}\sigma_{ik}(z-\tau_i)^{k-j-1} . \tag{60}$$

Putting $j' = j - k$,

$$\frac{q(z)}{w(z)} = \sum_{i=1}^{n} \sum_{k=0}^{s_i-1} \sum_{j'=0}^{s_i-1-k} \gamma_{i,j'+k}\sigma_{ik}(z-\tau_i)^{-j'-1} \tag{61}$$

Interchanging the second and third sums again and dropping the $'$,

$$\frac{q(z)}{w(z)} = \sum_{i=1}^{n} \sum_{j=0}^{s_i-1} \left(\sum_{k=0}^{si-1-j} \gamma_{i,j+k}\sigma_{ik} \right) (z-\tau_i)^{-j-1} \tag{62}$$

as claimed.

Now,

$$\alpha_{i,s_i-1} = \sum_{k=0}^{0} \gamma_{i,s_i-1+k}\sigma_{i,k} = \gamma_{i,s_i-1}\sigma_{i,0} \neq 0 , \tag{63}$$

also as claimed, since $\sigma_{i,0} = q(\tau_i) \neq 0$ □

Lemma 4 *If* $\deg q(z) \leqslant -2 - m + \sum_{i=1}^{n} s_i$*, then for all polynomials* $B(z)$ *of degree* $\leqslant m$ *and all polynomials* $f(z)$ *of degree* $\leqslant -2-m+\sum_{i=1}^{n} s_i$*, if the contour* C *is taken large enough to enclose all* τ_i

$$0 = \frac{1}{2\pi i} \oint_C \frac{B(z)f(z)}{w(z)} dz = \frac{1}{2\pi i} \oint_C \frac{B(z)q(z)}{w(z)} \cdot \frac{f(z)}{q(z)} dz . \tag{64}$$

Proof The proof follows by degree counting and Lemma 1. □

The idea of Theorem 2 can be generalized to the rational polynomial case.

Proposition 1 *Let, as before,* $R(z) = f(z)/q(z)$ *be the rational polynomial with* $q(z)$ *fixed. If* $B(z)$ *can be chosen as* $B^{IJ}(z) = \sum_{k=0}^{m-1} b_k^{IJ} z^k$ *so that*

$$\frac{B^{IJ}(z)q(z)}{w(z)} = \frac{-1}{(z-\tau_I)^{J+1}} + \sum_{i=1}^{n} \sum_{j \in S_i} \frac{\alpha_{ij}^{IJ}}{(z-\tau_i)^{j+1}} , \tag{65}$$

Fix the notation, we have avoided using the notation S_I^c *before the following* $\surd$

where $J \notin S_I$*, and as before* m *is the number of missing data items, then*

$$\frac{R^{(J)}(\tau_i)}{J!} = \sum_{i=1}^{n} \sum_{j \in S_i} \alpha_{ij}^{IJ} \rho_{ij} \tag{66}$$

for every polynomial $f(z)$ *of degree* $\leqslant -1-m+\sum_{i=1}^{n} S_i$ *and with*

$$\frac{R^{(j)}(\tau_i)}{j!} = \rho_{ij} \tag{67}$$

given for $1 \leqslant i \leqslant n$, $j \in S_i$ *. Recall also that for an arbitrary* ι, $R^{(\iota)}(\tau_i) = \frac{d^\iota}{dz^\iota} \left(\frac{f(z)}{q(z)} \right) \Big|_{\{z=\tau_i\}}$.

Proof Replace m with $m-1$ in Lemma 4 (note that the residues when $q(z)=0$ are zero), and apply Cauchy's Theorem, it follows that

$$\begin{aligned} 0 =& \frac{1}{2\pi i}\oint \frac{B(z)q(z)}{w(z)} \cdot \frac{f(z)}{q(z)} dz \\ =& \frac{1}{2\pi i}\oint \left(\frac{-1}{(z-\tau_I)^{(J+1)}} + \sum_{i=1}^{n}\sum_{j\in S_i} \frac{\alpha_{ij}^{IJ}}{(z-\tau_i)^{j+1}} \right) \frac{f(z)}{q(z)} dz \\ =& \frac{-R^{(J)}(\tau_i)}{J!} + \sum_{i=1}^{n}\sum_{j\in S_i} \alpha_{ij}^{IJ}\rho_{ij}\,. \end{aligned} \tag{68}$$

□

5 Conditioning, well-posedness and poisedness

6 Concluding remarks

(connection to divided differences)

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