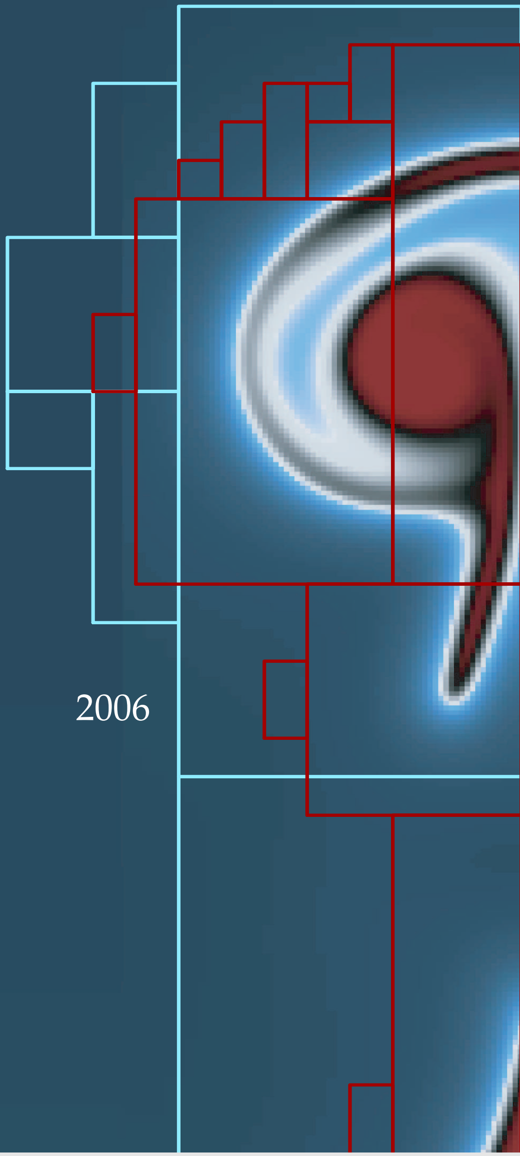
Communications in Applied Mathematics and Computational Science

Volume 1 No. 1 2006



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mathematical sciences publishers

COMM. APP. MATH. AND COMP. SCI.
Vol. 1, No. 1, 2006

ON INTERPOLATION AND INTEGRATION IN FINITE-DIMENSIONAL SPACES OF BOUNDED FUNCTIONS

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We observe that, under very mild conditions, an n-dimensional space of functions (with a finite n) admits numerically stable n-point interpolation and integration formulae. The proof relies entirely on linear algebra, and is virtually independent of the domain and of the functions to be interpolated.

1. Introduction

Approximation of functions and construction of quadrature formulae constitute an extremely well-developed area of numerical analysis; in most situations one is likely to encounter in practice, standard tools are satisfactory. Much of the research concentrates on obtaining powerful results under strong assumptions — designing interpolation and quadrature formulae for smooth functions on subspaces of $\mathbb{R}^n$, manifolds, etc. In this note, we make a very general observation that, given a finite set of bounded functions $f_1, f_2, \ldots, f_{n-1}, f_n$ (either real- or complex-valued) defined on a set S, there exists an interpolation formula that is exact on all linear combinations of $f_1, f_2, \ldots, f_{n-1}, f_n$, is numerically stable, and is based on n nodes in S (to be denoted $x_1, x_2, \ldots, x_{n-1}, x_n$). If, in addition, S is a measure space and the functions $f_1, f_2, \ldots, f_{n-1}, f_n$ are integrable, then there exists a quadrature formula based on the nodes $x_1, x_2, \ldots, x_{n-1}, x_n$ that is exact on all the functions $f_1, f_2, \ldots, f_{n-1}, f_n$, and is also numerically stable. Both of these statements are purely linear-algebraic in nature, and do not depend on the detailed properties of S, or of the functions $f_1, f_2, \ldots, f_{n-1}, f_n$.

It should be pointed out that all of the statements in this note follow easily from the analysis found in [4]; moreover, Theorem 2 can be found (in a slightly different form) in [7] and in [3]. Due to [3], the points used for interpolation in Theorem 2 are often called (nonelliptic) Fekete points, at least when the functions to be interpolated are polynomials. While we cannot cite earlier works where these

MSC2000: 65-02, ,

Keywords: interpolation, numerical integration, quadrature.

The authors were partially supported by the U.S. DoD under AFOSR Award #5710001605 and AFOSR Grant #F49620–03–C–0041, and by the U.S. NSF under Award #DMS–0139914.

observations are published, it seems unlikely that they had not been made a long time ago (perhaps in contexts other than numerical analysis).

This note has the following structure: Section 2 defines notation used in later sections, Section 3 provides a numerically stable interpolation scheme, Section 4 provides a numerically stable quadrature scheme, Section 5 provides a stronger result on the numerical stability of the interpolation scheme from Section 3, and Section 6 provides a couple of extensions to the techniques described in this note.

2. Notation

Throughout this note, S denotes an arbitrary set, n denotes a positive integer, and $f_1, f_2, \ldots, f_{n-1}, f_n$ denote bounded complex-valued functions on S (all results of this note also apply in the real-valued case, provided that the word "complex" is replaced with "real" everywhere). For any n points $x_1, x_2, \ldots, x_{n-1}, x_n$ in S, we define $A = A(x_1, x_2, \ldots, x_{n-1}, x_n)$ to be the $n \times n$ matrix defined via the formula

$$A_{j,k} = f_j(x_k) \tag{1}$$

with $j, k = 1, 2, \ldots, n-1, n$; we define the function g_k on S to be the ratio of the determinant of $A(x_1, x_2, \ldots, x_{k-2}, x_{k-1}, \; x, \; x_{k+1}, x_{k+2}, \ldots, x_{n-1}, x_n)$ to the determinant of $A(x_1, x_2, \ldots, x_{n-1}, x_n)$, via the formula

$$g_k(x) = \frac{\det A(x_1, x_2, \ldots, x_{k-2}, x_{k-1}, \; x, \; x_{k+1}, x_{k+2}, \ldots, x_{n-1}, x_n)}{\det A(x_1, x_2, \ldots, x_{n-1}, x_n)} \tag{2}$$

(here, the numerator is the same as the denominator, but with x in place of x_k). We define $D(x_1, x_2, \ldots, x_{n-1}, x_n)$ to be the modulus of the determinant of $A(x_1, x_2, \ldots, x_{n-1}, x_n)$, via the formula

$$D(x_1, x_2, \ldots, x_{n-1}, x_n) = \left| \det A(x_1, x_2, \ldots, x_{n-1}, x_n) \right|. \tag{3}$$

We define B to be the supremum of $D(x_1, x_2, \ldots, x_{n-1}, x_n)$ taken over all sets of n points $x_1, x_2, \ldots, x_{n-1}, x_n$ in S, via the formula

$$B = \sup_{x_1, x_2, \ldots, x_{n-1}, x_n \text{ in } S} D(x_1, x_2, \ldots, x_{n-1}, x_n). \tag{4}$$

For any x in S, we define $u = u(x)$ to be the $n \times 1$ column vector defined via the formula

$$u_k = f_k(x) \tag{5}$$

with $k = 1, 2, \ldots, n-1, n$, and we define $v = v(x)$ to be the $n \times 1$ column vector defined via the formula

$$v_k = g_k(x) \tag{6}$$

with $k = 1, 2, \ldots, n-1, n$.

3. Interpolation

Theorem 2 below asserts the existence of numerically stable n-point interpolation formulae for any set of n bounded functions; first we will need the following lemma.

Lemma 1. *Suppose that n is a positive integer, S is an arbitrary set containing at least n points, and $f_1, f_2, \dots, f_{n-1}, f_n$ are complex-valued functions on S that are linearly independent.*

Then, there exist n points $x_1, x_2, \dots, x_{n-1}, x_n$ in S such that the vectors $u(x_1)$, $u(x_2), \dots, u(x_{n-1}), u(x_n)$ defined in (5) are linearly independent.

Proof. We apply the modified Gram–Schmidt process (see, for example, [2]) to the set of all $n \times 1$ column vectors $u(x)$ defined in (5) for all x in S, while ensuring that all pivot vectors are nonzero via appropriate column-pivoting. □

Theorem 2. *Suppose that S is an arbitrary set, n is a positive integer, $f_1, f_2, \dots, f_{n-1}, f_n$ are bounded complex-valued functions on S, and ε is a positive real number such that*

$$\varepsilon \le 1. \tag{7}$$

Then, there exist n points $x_1, x_2, \dots, x_{n-1}, x_n$ in S and n functions $g_1, g_2, \dots, g_{n-1}, g_n$ on S such that

$$|g_k(x)| \le 1 + \varepsilon \tag{8}$$

for all x in S and $k = 1, 2, \dots, n-1, n$, and

$$f(x) = \sum_{k=1}^{n} f(x_k)\, g_k(x) \tag{9}$$

for all x in S and any function f defined on S via the formula

$$f(x) = \sum_{k=1}^{n} c_k\, f_k(x), \tag{10}$$

for some complex numbers $c_1, c_2, \dots, c_{n-1}, c_n$.

Proof. Without loss of generality, we assume that the functions $f_1, f_2, \dots, f_{n-1}, f_n$ are linearly independent.

Then, due to Lemma 1, B defined in (4) is strictly positive. Since the functions $f_1, f_2, \dots, f_{n-1}, f_n$ are bounded, $D(x_1, x_2, \dots, x_{n-1}, x_n)$ (defined in (3)) is also bounded, and hence the supremum B is not only strictly positive, but also finite. Therefore, by the definition of a supremum, there exist n points $x_1, x_2, \dots, x_{n-1}, x_n$ in S such that

$$B - D(x_1, x_2, \dots, x_{n-1}, x_n) \le \frac{B}{2}\varepsilon \tag{11}$$

and $D(x_1, x_2, \dots, x_{n-1}, x_n)$ is strictly positive.

Defining $g_1, g_2, \dots, g_{n-1}, g_n$ via (2), we obtain (9) from the Cramer rule applied to the linear system

$$Av = u, \tag{12}$$

where $A = A(x_1, x_2, \dots, x_{n-1}, x_n)$ is defined in (1), $v = v(x)$ is defined in (6), and $u = u(x)$ is defined in (5). Due to the combination of (11) and (7),

$$\frac{B}{2} \le D(x_1, x_2, \dots, x_{n-1}, x_n), \tag{13}$$

and due to the combination of (11) and (13),

$$\frac{B}{D(x_1, x_2, \dots, x_{n-1}, x_n)} - 1 \le \varepsilon; \tag{14}$$

we also observe that, due to (4),

$$D(x_1, x_2, \dots, x_{k-2}, x_{k-1}, \; x, \; x_{k+1}, x_{k+2}, \dots, x_{n-1}, x_n) \le B \tag{15}$$

for all x in S. Now, (8) is an immediate consequence of (2), (3), (15), (14). □

Remark 3. Due to (8), the interpolation formula (9) is numerically stable.

Remark 4. When calculations are performed using floating-point arithmetic, it is often desirable to "normalize" the set of functions $f_1, f_2, \dots, f_{n-1}, f_n$ before applying Theorem 2, by replacing this set with the set of functions $\tilde{f}_1, \tilde{f}_2, \dots, \tilde{f}_{n-1}, \tilde{f}_n$, where $\tilde{f}_k$ is the function defined on S via the formula

$$\tilde{f}_k(x) = \frac{f_k(x)}{\sum_{j=1}^{n} |f_j(x)|}, \tag{16}$$

for example.

Remark 5. The proof of Theorem 2 does not specify a computational means for choosing the points $x_1, x_2, \dots, x_{n-1}, x_n$ so that (11) is satisfied (that is, so that the interpolation scheme from Theorem 2 and the quadrature scheme from Theorem 8 are guaranteed to be numerically stable). However, combining the algorithms described in [1], [4] with appropriate discretizations of S yields methods for choosing the points that are proven to work, both in theory and in practice.

Remark 6. It is not hard to see that, if m is a positive integer with $m < n$ such that any set of strictly more than m of the n functions $f_1, f_2, \dots, f_{n-1}, f_n$ is linearly dependent, then only m summands are required in (9); all but m of the functions $g_1, g_2, \dots, g_{n-1}, g_n$ can be arranged to vanish identically at all points in their domain S. Slight variations on the algorithms in [5], [6] yield efficient, effective computational methods for taking full advantage of this fact. For an application of this fact, see [1].

Remark 7. When S is compact and the functions $f_1, f_2, \dots, f_{n-1}, f_n$ are continuous, Theorem 2 holds with $\varepsilon = 0$ rather than $\varepsilon > 0$, since a continuous function D on a compact space attains its maximal value. Analogously, Theorem 2 holds with $\varepsilon = 0$ when $S = \mathbb{R}^d$ for some positive integer d, the functions $f_1, f_2, \dots, f_{n-1}, f_n$ are continuous, and $f_k(x) \to 0$ as $|x| \to \infty$ for all $k = 1, 2, \dots, n-1, n$.

4. Quadratures

The following theorem formalizes the obvious observation that integrating both sides of (9) yields numerically stable quadrature formulae.

Theorem 8. *Suppose that S is a measure space, w is a nonnegative real-valued integrable function on S (that serves as the weight for integration), n is a positive integer, $f_1, f_2, \dots, f_{n-1}, f_n$ are bounded complex-valued integrable functions on S, and $\varepsilon \le 1$ is a positive real number.*

Then, there exist n complex numbers $w_1, w_2, \dots, w_{n-1}, w_n$ such that

$$|w_k| \le (1+\varepsilon) \int w(x)\, dx \tag{17}$$

for all $k = 1, 2, \dots, n-1, n$, and

$$\int f(x)\, w(x)\, dx = \sum_{k=1}^{n} w_k\, f(x_k) \tag{18}$$

for any function f defined on S via (10), where $x_1, x_2, \dots, x_{n-1}, x_n$ are the n points in S chosen in Theorem 2.

Proof. For each $k = 1, 2, \dots, n-1, n$, we define w_k via the formula

$$w_k = \int g_k(x)\, w(x)\, dx, \tag{19}$$

where $g_1, g_2, \dots, g_{n-1}, g_n$ are the functions from Theorem 2. Then, (17) is an immediate consequence of (19) and (8). Moreover, (18) is an immediate consequence of (9) and (19). □

Remark 9. Needless to say, the weight function w in the above theorem is superfluous; it could be absorbed into the measure on S. However, we found the formulations of Theorems 8 and 12 involving w to be convenient in applications. While Theorems 8 and 12 require the functions $f_1, f_2, \dots, f_{n-1}, f_n$ to be bounded (perhaps after "normalizing" them as in Remark 4 or otherwise rescaling them), these theorems do not require the weight function w to be bounded.

Remark 10. Theorem 8 asserts the existence under very mild conditions of numerically stable quadratures that integrate linear combinations of n functions using the values of these linear combinations tabulated at n appropriately chosen points. In contrast, construction of optimal "generalized Gaussian" quadratures, which tabulate the linear combinations at fewer nodes than the number of functions, requires more subtle techniques (see, for example, the references cited in [8]).

5. Strengthened numerical stability

Theorem 2 provides the bound (8) under the rather weak assumption that the functions $f_1, f_2, \dots, f_{n-1}, f_n$ are bounded (in fact, this assumption is necessary for (8)). Theorem 12 below provides a stronger bound under the additional assumption that there exists a measure with respect to which the functions $f_1, f_2, \dots, f_{n-1}$, f_n are orthonormal. This stronger bound can be obtained by first using Theorem 2 to reconstruct the function f defined in (10) on its entire domain S from its values $f(x_1), f(x_2), \dots, f(x_{n-1}), f(x_n)$, as per (9). Then, the coefficients c_1, $c_2, \dots, c_{n-1}, c_n$ in (10) can be calculated by taking the appropriate inner products with the reconstruction of f just obtained. Finally, f can be reconstructed on its entire domain S via (10), using the values of $c_1, c_2, \dots, c_{n-1}, c_n$ just obtained, and the values $f_1(x), f_2(x), \dots, f_{n-1}(x), f_n(x)$, which are assumed to be known for any x in S. (However, please note that the proof of Theorem 12 given below follows this prescription only implicitly.) First, we will need the following lemma, stating that the relation (9) determines the functions $g_1, g_2, \dots, g_{n-1}, g_n$ uniquely, provided that the functions $f_1, f_2, \dots, f_{n-1}, f_n$ are linearly independent.

Lemma 11. *Suppose that n is a positive integer, S is an arbitrary set containing at least n points, $f_1, f_2, \dots, f_{n-1}, f_n$ are bounded complex-valued functions on S, and $\varepsilon \le 1$ is a positive real number. Suppose in addition that $f_1, f_2, \dots, f_{n-1}$, f_n are linearly independent, and that $h_1, h_2, \dots, h_{n-1}, h_n$ are functions on S such that*

$$f(x) = \sum_{k=1}^{n} f(x_k)\, h_k(x) \tag{20}$$

for all x in S and any function f defined on S via (10), where $x_1, x_2, \dots, x_{n-1}$, x_n are the n points in S chosen in Theorem 2.

Then,

$$h_k(x) = g_k(x) \tag{21}$$

for all x in S and $k = 1, 2, \dots, n-1, n$, where $g_1, g_2, \dots, g_{n-1}, g_n$ are defined in (2).

Proof. For any x in S, due to (20),

$$At = u, \tag{22}$$

where $A = A(x_1, x_2, \ldots, x_{n-1}, x_n)$ is defined in (1), $u = u(x)$ is defined in (5), and $t = t(x)$ is defined to be an $n \times 1$ column vector via the formula

$$t_k = h_k(x) \tag{23}$$

with $k = 1, 2, \ldots, n-1, n$; subtracting (12) from (22),

$$A(t - v) = 0, \tag{24}$$

where $v = v(x)$ is defined in (6). Due to Lemma 1, B defined in (4) is strictly positive, so that A defined in (1) is invertible, and therefore, due to (24),

$$t(x) = v(x) \tag{25}$$

for all x in S. Then, (21) is an immediate consequence of (25), (23), (6). □

Theorem 12. *Suppose that n is a positive integer, S is a measure space containing at least n points, w is a nonnegative real-valued integrable function on S (that serves as the weight for integration), $f_1, f_2, \ldots, f_{n-1}, f_n$ are bounded complex-valued square-integrable functions on S, and $\varepsilon \le 1$ is a positive real number. Suppose further that $f_1, f_2, \ldots, f_{n-1}, f_n$ are orthonormal, that is,*

$$\int |f_k(x)|^2 \, w(x) \, dx = 1 \tag{26}$$

for all $k = 1, 2, \ldots, n-1, n$, and

$$\int \overline{f_j(x)} \, f_k(x) \, w(x) \, dx = 0 \tag{27}$$

whenever $j \ne k$.

Then,

$$|g_k(x)| \le (1+\varepsilon) \sqrt{\int w(y) \, dy} \, \sum_{j=1}^{n} |f_j(x)| \tag{28}$$

for all x in S and $k = 1, 2, \ldots, n-1, n$, where $g_1, g_2, \ldots, g_{n-1}, g_n$ are defined in (2), with the n points $x_1, x_2, \ldots, x_{n-1}, x_n$ in S chosen in Theorem 2.

Proof. In order to prove (28), for each $k = 1, 2, \ldots, n-1, n$, we define the function h_k on S via the formula

$$h_k(x) = \sum_{j=1}^{n} f_j(x) \int \overline{f_j(y)} \, g_k(y) \, w(y) \, dy \tag{29}$$

and demonstrate both that (21) holds with the functions $h_1, h_2, \ldots, h_{n-1}, h_n$ defined in (29), and that

$$|h_k(x)| \le (1+\varepsilon) \sqrt{\int w(y)\,dy} \sum_{j=1}^{n} |f_j(x)| \tag{30}$$

for all x in S and $k = 1, 2, \ldots, n-1, n$.

We first show that (21) holds with the functions $h_1, h_2, \ldots, h_{n-1}, h_n$ defined in (29), by demonstrating that $h_1, h_2, \ldots, h_{n-1}, h_n$ satisfy the hypotheses of Lemma 11. Suppose that f is defined via (10). To verify that (20) holds with the functions $h_1, h_2, \ldots, h_{n-1}, h_n$ defined in (29), we substitute (29) into the right hand side of (20) and exchange the orders of summation and integration, obtaining that

$$\sum_{k=1}^{n} f(x_k)\, h_k(x) = \sum_{j=1}^{n} f_j(x) \int \overline{f_j(y)} \sum_{k=1}^{n} f(x_k)\, g_k(y)\, w(y)\, dy \tag{31}$$

for all x in S. Due to the combination of (31) and (9),

$$\sum_{k=1}^{n} f(x_k)\, h_k(x) = \sum_{j=1}^{n} f_j(x) \int \overline{f_j(y)}\, f(y)\, w(y)\, dy \tag{32}$$

for all x in S. Then, (20) is an immediate consequence of applying (10), (26), and (27) to the right hand side of (32).

Furthermore, the functions $f_1, f_2, \ldots, f_{n-1}, f_n$ are linearly independent, since they are assumed to be orthonormal. Thus, all of the hypotheses of Lemma 11 are satisfied, so (21) holds with the functions $h_1, h_2, \ldots, h_{n-1}, h_n$ defined in (29).

Finally, due to the Cauchy–Schwarz inequality,

$$\left| \int \overline{f_k(y)}\, g_k(y)\, w(y)\, dy \right| \le \sqrt{\int |f_k(y)|^2\, w(y)\, dy} \sqrt{\int |g_k(y)|^2\, w(y)\, dy}, \tag{33}$$

and, due to (8),

$$\sqrt{\int |g_k(y)|^2\, w(y)\, dy} \le (1+\varepsilon) \sqrt{\int w(y)\, dy} \tag{34}$$

for all $k = 1, 2, \ldots, n-1, n$. Then, (30) is an immediate consequence of (29), (33), (26), (34), and then (28) is an immediate consequence of (21) and (30). □

Remark 13. Due to (28), the interpolation formula (9) is numerically stable. While the numerical stability guaranteed by (8) is sufficient under most conditions, sometimes the bound (28) is more useful. The bound (28) is stronger than the bound (8) in the sense that, if all of the values $|f_1(x)|, |f_2(x)|, \ldots, |f_{n-1}(x)|, |f_n(x)|$ are small at some point x in S, then all of the values $|g_1(x)|$, $|g_2(x)|$, ..., $|g_{n-1}(x)|$, $|g_n(x)|$ are accordingly small at that point x.

Remark 14. Theorem 12 generalizes easily to the case when the functions f_1, f_2, ..., f_{n-1}, f_n are not precisely orthonormal, but only "close" to orthonormal, in the sense that the condition number of their Gram matrix is reasonably small.

6. Concluding remarks

The following remarks pertain to some fairly obvious but nonetheless useful extensions of the techniques described in this note.

Remark 15. One often encounters infinite-dimensional spaces of functions that are finite-dimensional to a specified precision. A typical situation of this kind involves the range of a compact operator, and the usual way to construct the finite-dimensional approximation is via the Singular Value Decomposition (see, for example, [8]). When combined with this observation, the apparatus of the present note becomes applicable to many infinite-dimensional spaces of functions.

Remark 16. In numerical practice, rather than dealing directly with functions that have finite mass or finite energy but are nevertheless unbounded, we often instead treat the bounded functions obtained from the unbounded ones via either spectral/pseudospectral transforms or localized averaging (involving convolution with kernels that are bounded or have finite energy, for example).

7. Acknowledgements

We would like to thank Reiji Suda and Masaaki Sugihara for pointing out the standard term "Fekete points". In addition, we would like to thank the anonymous reviewers for helpful editorial suggestions.

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Received December 10, 2005.

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