

Recurrence Relations and Fast Algorithms

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Abstract

We construct fast algorithms for decomposing into and reconstructing from linear combinations of functions which satisfy recurrence relations (such decompositions and reconstructions are also known as analysis and synthesis of series of special functions). The algorithms are efficient in the sense that there exists a positive real number C such that, for any positive integer n and positive real number ε , the algorithms require at most $C n (\ln n) \ln(1/\varepsilon)$ operations and memory storage elements to evaluate at n appropriately chosen points any specified linear combination of n special functions, to a precision of approximately ε .

1 Introduction

Over the past several decades, the Fast Fourier Transform (FFT) and its variants (see, for example, [8]) have had an enormous impact across the sciences. The FFT is an efficient algorithm for computing, for any even positive integer n and complex numbers $\beta_1, \beta_2, \dots, \beta_{n-1}, \beta_n$, the complex numbers $\alpha_1, \alpha_2, \dots, \alpha_{n-1}, \alpha_n$ defined by

$$\alpha_j = \sum_{k=1}^n \beta_k f_k(x_j) \quad (1)$$

for $j = 1, 2, \dots, n-1, n$, where $f_1, f_2, \dots, f_{n-1}, f_n$ are the functions defined on $[-1, 1]$ by

$$f_k(x) = \exp\left(\frac{\pi i (2k - n) x}{2}\right) \quad (2)$$

for $k = 1, 2, \dots, n-1, n$, and $x_1, x_2, \dots, x_{n-1}, x_n$ are the real numbers defined by

$$x_k = \frac{2k - n}{n} \quad (3)$$

for $k = 1, 2, \dots, n-1, n$. The FFT is efficient in the sense that there exists a reasonably small positive real number C such that, for any positive integer n , the FFT requires at most $C n \ln n$ operations and memory storage elements to compute $\alpha_1, \alpha_2, \dots, \alpha_{n-1}, \alpha_n$ in (1) from $\beta_1, \beta_2, \dots, \beta_{n-1}, \beta_n$. In contrast, evaluating the sum in (1) separately for every $j = 1, 2, \dots, n-1, n$ costs at least n^2 operations in total.

The present paper introduces similarly efficient algorithms for computing $\alpha_1, \alpha_2, \dots, \alpha_{n-1}, \alpha_n$ in (1) from $\beta_1, \beta_2, \dots, \beta_{n-1}, \beta_n$, and (when appropriate) for the inverse procedure of computing $\beta_1, \beta_2, \dots, \beta_{n-1}, \beta_n$ from $\alpha_1, \alpha_2, \dots, \alpha_{n-1}, \alpha_n$, for more general collections of functions $f_1, f_2, \dots, f_{n-1}, f_n$ and points $x_1, x_2, \dots, x_{n-1}, x_n$ than those defined in (2) and (3). Specifically, the present paper constructs algorithms for classes of functions which satisfy recurrence relations. The present paper describes in detail a few representative examples of such classes of functions, namely weighted orthonormal polynomials and Bessel functions of varying orders. These collections of functions satisfy recurrence relations of the form

$$g(x) f_k(x) = c_{k-1} f_{k-1}(x) + d_k f_k(x) + c_k f_{k+1}(x) \quad (4)$$

for all x in the domain, where c_{k-1}, c_k , and d_k are real numbers and either $g(x) = x$ or $g(x) = \frac{1}{x}$; c_k, d_k , and g vary with the collection of functions under consideration.

The fast algorithms all rely on the following two observations:

1. The solutions to the recurrence relation in (4) are the eigenvectors corresponding to eigenvalues $g(x)$ of certain tridiagonal real self-adjoint matrices. The tridiagonal real self-adjoint matrices required are usually infinite-dimensional, but turn out to be finite-dimensional for special values of x in (4).
2. There exist fast algorithms for determining and applying matrices whose columns are normalized eigenvectors of a tridiagonal real self-adjoint matrix, and for applying the adjoints of these matrices of eigenvectors.

The first observation has been well known to numerical analysts at least since the seminal [4] appeared; the second observation has been reasonably well known to numerical analysts since the seminal [6] appeared. However, the combination seems to be new.

The methods described in the present paper should lead to fairly efficient codes for computing a variety of what are known as pseudospectral transforms. In particular, we outline in Remark 34 how to use the methods to construct fast algorithms for decomposing into and reconstructing from linear combinations of spherical harmonics.

We refer to [10] and its compilation of references for prior work on related fast algorithms, as well as to [7] for an alternative approach suitable for some applications. The present paper simply introduces techniques that are substantially more efficient than the very similar ones described in [10]. We intend to report separately carefully optimized implementations of the theory described in the present paper.

The present paper has the following structure: Subsection 2.1 summarizes the properties of fast algorithms for spectral representations of tridiagonal real self-adjoint matrices, Subsection 2.2 reiterates facts having to do with recurrence relations for orthonormal polynomials, Subsection 2.3 reiterates facts having to do with recurrence relations for Bessel functions, and Section 3 employs the subsections of Section 2 to construct fast algorithms for various purposes.

2 Preliminaries

This section summarizes widely known facts from numerical and mathematical analysis in the corresponding subsections. Section 3 uses the results of the present section to construct

fast algorithms.

2.1 Divide-and-conquer spectral methods

This subsection summarizes in Remark 1 the properties of fast algorithms introduced in [5] and [6] for spectral representations of tridiagonal real self-adjoint matrices.

Remark 1 As first introduced in [6], there exist a real number C and well-conditioned algorithms A_1, A_2, A_3, A_4 , and A_5 such that, for any positive real number ε , positive integer n , tridiagonal real self-adjoint $n \times n$ matrix T with n distinct eigenvalues, real unitary matrix U whose columns are n normalized eigenvectors of T , and real $n \times 1$ column vector v ,

1. A_1 computes to precision $\|T\| \varepsilon$ the n eigenvalues of T , using at most $C n (\ln n) \ln(1/\varepsilon)$ operations and memory storage elements,
2. A_2 computes to precision $(\sqrt{n} \|T\| \varepsilon)/\delta$ the n entries of the matrix-vector product $U v$, using at most $C n (\ln n) \ln(1/\varepsilon)$ operations and storage elements,
3. A_3 computes to precision $(\sqrt{n} \|T\| \varepsilon)/\delta$ the n entries of the matrix-vector product $U^T v$, using at most $C n (\ln n) \ln(1/\varepsilon)$ operations and storage elements, and,
4. after A_4 performs some precomputations which are particular to T at a cost of at most $C n (\ln n) \ln(1/\varepsilon)$ operations and storage elements, A_5 computes to precision $(\sqrt{n} \|T\| \varepsilon)/\delta$ the kn entries of any k eigenvectors of T , using at most $C k n \ln(1/\varepsilon)$ operations and storage elements, for any positive integer k ,

where $\|T\|$ is the absolute value of the largest eigenvalue of T , and δ is the minimum value of the distance $|\lambda - \mu|$ between any two distinct eigenvalues λ and μ of T ($\lambda \neq \mu$).

Remark 2 There exist algorithms with properties very similar to those mentioned in Remark 1 when the eigenvalues of T are not all distinct.

2.2 Orthonormal polynomials

This subsection discusses rather classical facts concerning orthonormal polynomials. All of these facts follow trivially from results contained, for example, in [11]. The well-known [4] utilizes an entirely similar collection of facts to construct algorithms related to those described in the present paper in Subsection 3.1.

Subsections 3.1 and 3.3 employ Lemmas 7, 8, and 9, which formulate certain simple consequences of Theorems 3 and 6. Lemmas 5 and 16 provide the results of some calculations for what are known as normalized Jacobi polynomials, a classical example of a family of orthonormal polynomials; the results of analogous calculations for some other classical families of polynomials appear to exhibit similar behaviors. The remaining lemmas in the present subsection, Lemmas 11 and 14, deal with certain conditioning issues surrounding the algorithms in Subsections 3.1 and 3.3 (see Remark 15). The remaining theorem in the present subsection, Theorem 13, describes what are known as Gauss-Jacobi quadrature formulae.

In the present subsection, we index vectors and matrices starting at entry 0.

We say that a is an extended real number to mean that a is a real number, $a = +\infty$, or $a = -\infty$. For any real number a , we define the intervals $[a, \infty] = [a, \infty)$ and $[-\infty, a] = (-\infty, a]$; we define $[-\infty, \infty] = (-\infty, \infty)$.

For any extended real numbers a and b with $a < b$ and nonnegative integer n , we say that $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$ for a weight w to mean that w is a real-valued nonnegative integrable function on $[a, b]$, p_k is a polynomial of degree k , the coefficients of $x^0, x^1, \dots, x^{k-1}, x^k$ in $p_k(x)$ are real, and the coefficient of x^k in $p_k(x)$ is positive for $k = 0, 1, \dots, n-1, n$, and

$$\int_a^b dx w(x) p_j(x) p_k(x) = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases} \quad (5)$$

for $j, k = 0, 1, \dots, n-1, n$.

The following theorem states that a system of orthonormal polynomials satisfy a certain three-term recurrence relation.

Theorem 3 *Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$.*

Then, there exist real numbers $c_0, c_1, \dots, c_{n-2}, c_{n-1}$ and $d_0, d_1, \dots, d_{n-2}, d_{n-1}$ such that

$$x p_0(x) = d_0 p_0(x) + c_0 p_1(x) \quad (6)$$

for any $x \in [a, b]$, and

$$x p_k(x) = c_{k-1} p_{k-1}(x) + d_k p_k(x) + c_k p_{k+1}(x) \quad (7)$$

for any $x \in [a, b]$ and $k = 1, 2, \dots, n-2, n-1$.

Proof. Theorem 3.2.1 in [11] provides an equivalent formulation of the present theorem. \square

Remark 4 In fact, $c_k > 0$ for $k = 0, 1, \dots, n-2, n-1$, in (6) and (7).

The following lemma provides expressions for $c_0, c_1, \dots, c_{n-2}, c_{n-1}$ and $d_0, d_1, \dots, d_{n-2}, d_{n-1}$ from (6) and (7) for what are known as normalized Jacobi polynomials.

Lemma 5 *Suppose that $a = -1, b = 1, \alpha$ and β are real numbers with $\alpha > -1$ and $\beta > -1$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are the orthonormal polynomials on $[a, b]$ for the weight w defined by*

$$w(x) = (1-x)^\alpha (1+x)^\beta. \quad (8)$$

Then,

$$c_k = \sqrt{\frac{4(k+1)(k+\alpha+1)(k+\beta+1)(k+\alpha+\beta+1)}{(2k+\alpha+\beta+1)(2k+\alpha+\beta+2)^2(2k+\alpha+\beta+3)}} \quad (9)$$

and

$$d_k = \frac{\beta^2 - \alpha^2}{(2k+\alpha+\beta)(2k+\alpha+\beta+2)} \quad (10)$$

for $k = 0, 1, \dots, n-2, n-1$, where $c_0, c_1, \dots, c_{n-2}, c_{n-1}$ and $d_0, d_1, \dots, d_{n-2}, d_{n-1}$ are from (6) and (7).

Proof. Formulae 4.5.1 and 4.3.4 in [11] together provide an equivalent formulation of the present lemma. \square

The following theorem states that the polynomial of degree n in a system of orthonormal polynomials on $[a, b]$ has n distinct zeros in $[a, b]$.

Theorem 6 *Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$.*

Then, there exist distinct real numbers $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ such that $x_k \in [a, b]$ and

$$p_n(x_k) = 0 \quad (11)$$

for $k = 0, 1, \dots, n-2, n-1$, and

$$x_j \neq x_k \quad (12)$$

when $j \neq k$ for $j, k = 0, 1, \dots, n-2, n-1$.

Proof. Theorem 3.3.4 in [11] provides a slightly more general formulation of the present theorem. \square

Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$ for a weight w . We define T to be the tridiagonal real self-adjoint $n \times n$ matrix with the entry

$$T_{j,k} = \begin{cases} c_{j-1}, & k = j - 1 \\ d_j, & k = j \\ c_j, & k = j + 1 \\ 0, & \text{otherwise (when } k < j - 1 \text{ or } k > j + 1) \end{cases} \quad (13)$$

for $j, k = 0, 1, \dots, n-2, n-1$, where $c_0, c_1, \dots, c_{n-2}, c_{n-1}$ and $d_0, d_1, \dots, d_{n-2}, d_{n-1}$ are from (6) and (7). For $k = 0, 1, \dots, n-1, n$, we define the function q_k on $[a, b]$ by

$$q_k(x) = \sqrt{w(x)} p_k(x). \quad (14)$$

We define U to be the real $n \times n$ matrix with the entry

$$U_{j,k} = \frac{q_j(x_k)}{\sqrt{\sum_{m=0}^{n-1} (q_m(x_k))^2}} \quad (15)$$

for $j, k = 0, 1, \dots, n-2, n-1$, where $q_0, q_1, \dots, q_{n-2}, q_{n-1}$ are defined in (14), and $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ are from (11). We define Λ to be the diagonal real $n \times n$ matrix with the entry

$$\Lambda_{j,k} = \begin{cases} x_j, & k = j \\ 0, & k \neq j \end{cases} \quad (16)$$

for $j, k = 0, 1, \dots, n-2, n-1$, where $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ are from (11). We define S to be the diagonal real $n \times n$ matrix with the entry

$$S_{j,k} = \begin{cases} \sqrt{\sum_{m=0}^{n-1} (q_m(x_j))^2}, & k = j \\ 0, & k \neq j \end{cases} \quad (17)$$

for $j, k = 0, 1, \dots, n-2, n-1$, where $q_0, q_1, \dots, q_{n-2}, q_{n-1}$ are defined in (14), and $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ are from (11). We define e to be the real $n \times 1$ column vector with the entry

$$e_k = \begin{cases} 1, & k = 0 \\ 0, & k \neq 0 \end{cases} \quad (18)$$

for $k = 0, 1, \dots, n-2, n-1$.

The following lemma states that U is a matrix of normalized eigenvectors of the tridiagonal real self-adjoint matrix T and that Λ is a diagonal matrix whose diagonal entries are the eigenvalues of T (which, according to (12), are distinct).

Lemma 7 *Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$ for a weight w .*

Then,

$$U^T T U = \Lambda, \quad (19)$$

where T is defined in (13), U is defined in (15), and Λ is defined in (16). Moreover, U is real and unitary.

Proof. Combining (6), (7), and (11) yields that

$$T U = U \Lambda. \quad (20)$$

Combining (20), (15), (16), and (12) yields that U is a real matrix of normalized eigenvectors of T , with distinct corresponding eigenvalues. Therefore, since eigenvectors corresponding to distinct eigenvalues of a real self-adjoint matrix are orthogonal, U is orthogonal. Applying U^T from the left to both sides of (20) yields (19). \square

The following lemma expresses in matrix notation the decompositions into and reconstructions from linear combinations of weighted orthonormal polynomials for which Subsection 3.3 describes fast algorithms.

Lemma 8 *Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$ for a weight w , and α and β are real $n \times 1$ column vectors such that α has the entry*

$$\alpha_j = \sum_{k=0}^{n-1} \beta_k q_k(x_j) \quad (21)$$

for $j = 0, 1, \dots, n-2, n-1$, where $q_0, q_1, \dots, q_{n-2}, q_{n-1}$ are defined in (14), and $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ are from (11).

Then,

$$\alpha = S U^T \beta \quad (22)$$

and

$$\beta = U S^{-1} \alpha, \quad (23)$$

where U is defined in (15) and S is defined in (17).

Proof. Combining (15) and (17) yields (22). According to Lemma 7, U is real and unitary. Therefore, applying $U S^{-1}$ from the left to both sides of (22) yields (23). \square

The following two lemmas provide alternative expressions for the entries of S defined in (17).

Lemma 9 *Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$ for a weight w .*

Then,

$$S_{k,k} = \frac{\sqrt{w(x_k)}}{(U^T e)_k \sqrt{\int_a^b dx w(x)}} \quad (24)$$

for $k = 0, 1, \dots, n-2, n-1$, where S is defined in (17), U is defined in (15), e is defined in (18), $(U^T e)_0, (U^T e)_1, \dots, (U^T e)_{n-2}, (U^T e)_{n-1}$ are the entries of the matrix-vector product $U^T e$, and $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ are from (11).

Proof. Combining (15) and (18) yields that

$$(U^T e)_k = \frac{q_0(x_k)}{\sqrt{\sum_{m=0}^{n-1} (q_m(x_k))^2}} \quad (25)$$

for $k = 0, 1, \dots, n-2, n-1$. Since the polynomial p_0 has degree 0, combining (5) and (14) yields that

$$q_0(x) = \frac{\sqrt{w(x)}}{\sqrt{\int_a^b dy w(y)}} \quad (26)$$

for any $x \in [a, b]$. Combining (17), (25), and (26) yields (24). \square

Remark 10 Formula 2.6 in [4] motivated us to employ the equivalent (24).

Lemma 11 *Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$ for a weight w , and k is a nonnegative integer such that $\ln w$ is differentiable at the point x_k from (11).*

Then,

$$(S_{k,k})^2 = c_{n-1} q_{n-1}(x_k) \frac{d}{dx} q_n(x_k), \quad (27)$$

where $S_{k,k}$ is defined in (17), c_{n-1} is from (7), q_{n-1} and q_n are defined in (14), and x_k is from (11).

Proof. Formula 3.2.4 in [11] provides a slightly more general formulation of the present lemma. \square

Remark 12 There exist similar formulations of Lemma 11 when it is not the case that $\ln w$ is differentiable at x_k .

The following theorem describes what are known as Gauss-Jacobi quadrature formulae for orthonormal polynomials.

Theorem 13 *Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$ for a weight w .*

Then, there exist positive real numbers $w_0, w_1, \dots, w_{n-2}, w_{n-1}$, called the Christoffel numbers for $x_0, x_1, \dots, x_{n-2}, x_{n-1}$, such that

$$\int_a^b dx w(x) p(x) = \sum_{k=0}^{n-1} w_k p(x_k) \quad (28)$$

for any polynomial p of degree at most $2n - 1$, where $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ are from (11).

Proof. Theorems 3.4.1 and 3.4.2 in [11] together provide a slightly more general formulation of the present theorem. \square

The following lemma provides alternative expressions for the entries of S defined in (17).

Lemma 14 *Suppose that a and b are extended real numbers with $a < b$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are orthonormal polynomials on $[a, b]$ for a weight w .*

Then,

$$(S_{k,k})^2 = \frac{w(x_k)}{w_k} \quad (29)$$

for $k = 0, 1, \dots, n - 2, n - 1$, where S is defined in (17), and $w_0, w_1, \dots, w_{n-2}, w_{n-1}$ are the Christoffel numbers from (28) for the corresponding points $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ from (11). Moreover, there exist extended real numbers $y_0, y_1, \dots, y_{n-1}, y_n$ such that $a = y_0 < y_1 < \dots < y_{n-1} < y_n = b$ and

$$w_k = \int_{y_k}^{y_{k+1}} dx w(x) \quad (30)$$

for $k = 0, 1, \dots, n - 2, n - 1$.

Proof. Formula 3.4.8 in [11] provides an equivalent formulation of (29). Formula 3.41.1 in [11] provides a slightly more a general formulation of (30). \square

Remark 15 The formulae (17), (27), (29), and (30) give some insight into the condition number of S . Due to (17), the entries of S are usually not too large. Due to (29) and (30), for each $k = 0, 1, \dots, n - 2, n - 1$, if the ratio

$$\frac{w(x_k)}{\int_a^b dx w(x)} \quad (31)$$

is exceedingly large, then $S_{k,k}$ is exceedingly large.

The following lemma provides an alternative expression for the entries of S defined in (17) for what are known as normalized Jacobi polynomials.

Lemma 16 *Suppose that $a = -1$, $b = 1$, α and β are real numbers with $\alpha > -1$ and $\beta > -1$, n is a positive integer, and $p_0, p_1, \dots, p_{n-1}, p_n$ are the orthonormal polynomials on $[a, b]$ for the weight w defined by*

$$w(x) = (1 - x)^\alpha (1 + x)^\beta. \quad (32)$$

Then,

$$S_{k,k} = \sqrt{\frac{1 - x_k^2}{2n + \alpha + \beta + 1}} \left| \frac{d}{dx} q_n(x_k) \right| \quad (33)$$

for $k = 0, 1, \dots, n - 2, n - 1$, where S is defined in (17), $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ are from (11), and q_n is defined in (14).

Proof. Together with (29), Formulae 15.3.1 and 4.3.4 in [11] provide an equivalent formulation of the present lemma. \square

2.3 Bessel functions

This subsection discusses well-known facts concerning Bessel functions. All of these facts follow trivially from results contained, for example, in [12] and [3].

Subsections 3.2 and 3.4 employ Lemmas 24, 25, 26, and 27, which formulate certain simple consequences of Theorems 18 and 21 and Corollary 22, by way of Lemmas 19 and 23. The remaining lemmas in the present subsection, Lemmas 31 and 32, provide closed-form results of some calculations for what are known as spherical Bessel functions, a family of Bessel functions frequently encountered in applications.

In the present subsection, we index vectors and matrices starting at entry 1.

Suppose that ν is a nonnegative real number. For any nonnegative integer k , we define the function f_k on $(0, \infty)$ by

$$f_k(x) = \frac{2^\nu \Gamma(\nu + 1) \sqrt{\nu + k}}{x^\nu} J_{\nu+k}(x), \quad (34)$$

where Γ is the gamma (factorial) function and $J_{\nu+k}$ is the Bessel function of the first kind of order $\nu + k$ (see, for example, [12]).

Remark 17 Formula 8 of Section 3.1 in [12] provides a slightly more general formulation of the fact that

$$\lim_{x \rightarrow 0^+} \frac{2^\nu \Gamma(\nu + 1)}{x^\nu} J_\nu(x) = 1, \quad (35)$$

which motivated our choice of normalization in (34).

The following theorem states that f_1, f_2, f_3, \dots defined in (34) satisfy a certain three-term recurrence relation.

Theorem 18 *Suppose that ν is a nonnegative real number.*

Then,

$$\frac{1}{x} f_1(x) = \frac{1}{2\sqrt{(\nu+1)}} \frac{2^\nu \Gamma(\nu+1)}{x^\nu} J_\nu(x) + \frac{1}{2\sqrt{(\nu+1)(\nu+2)}} f_2(x) \quad (36)$$

for any positive real number x , and

$$\frac{1}{x} f_k(x) = \frac{1}{2\sqrt{(\nu+k-1)(\nu+k)}} f_{k-1}(x) + \frac{1}{2\sqrt{(\nu+k)(\nu+k+1)}} f_{k+1}(x) \quad (37)$$

for any positive real number x and $k = 2, 3, 4, \dots$, where f_1, f_2, f_3, \dots are defined in (34), Γ is the gamma (factorial) function, and J_ν is the Bessel function of the first kind of order ν (see, for example, [12]).

Proof. Formula 1 of Section 3.2 in [12] provides a somewhat more general formulation of the present theorem. \square

Suppose that ν is a nonnegative real number and n is a positive integer. We define T to be the tridiagonal real self-adjoint $n \times n$ matrix with the entry

$$T_{j,k} = \begin{cases} \frac{1}{2\sqrt{(\nu+j-1)(\nu+j)}}, & k = j - 1 \\ \frac{1}{2\sqrt{(\nu+j)(\nu+j+1)}}, & k = j + 1 \\ 0, & \text{otherwise (when } k < j - 1, k = j, \text{ or } k > j + 1) \end{cases} \quad (38)$$

for $j, k = 1, 2, \dots, n - 1, n$. For any positive real number x , we define $v = v(x)$ to be the real $n \times 1$ column vector with the entry

$$v_k = \frac{f_k(x)}{\sqrt{\sum_{m=1}^n (f_m(x))^2}} \quad (39)$$

for $k = 1, 2, \dots, n - 1, n$, where $f_1, f_2, \dots, f_{n-1}, f_n$ are defined in (34). For any positive real number x , we define $\delta = \delta(x)$ to be the real number

$$\delta = \frac{1}{2\sqrt{(\nu+n)(\nu+n+1)}} \frac{|f_{n+1}(x)|}{\sqrt{\sum_{m=1}^n (f_m(x))^2}}, \quad (40)$$

where $f_1, f_2, \dots, f_n, f_{n+1}$ are defined in (34).

The following lemma states that v is nearly an eigenvector of the tridiagonal real self-adjoint matrix T corresponding to an approximate eigenvalue of $\frac{1}{x}$ for any positive real number x such that $J_\nu(x) = 0$ and δ is small.

Lemma 19 *Suppose that ν is a nonnegative real number and n is a positive integer.*

Then,

$$\left| (Tv)_n - \frac{1}{x} v_n \right| \leq \delta \quad (41)$$

and

$$(T v)_k = \frac{1}{x} v_k \quad (42)$$

for $k = 1, 2, \dots, n-2, n-1$ and any positive real number x with

$$J_\nu(x) = 0, \quad (43)$$

where T is defined in (38), $v = v(x)$ is defined in (39), $(T v)_1, (T v)_2, \dots, (T v)_{n-1}, (T v)_n$ are the entries of the matrix-vector product $T v$, $\delta = \delta(x)$ is defined in (40), and J_ν is the Bessel function of the first kind of order ν (see, for example, [12]).

Proof. Combining (37), (36), and (43) yields (41) and (42). \square

Remark 20 It is well known that, for any positive real number x , $J_{\nu+n+1}(x)$ and thence δ defined in (40) decays extremely rapidly as n increases past a band around $n = x$ of width proportional to $x^{1/3}$; see, for example, Lemma 2.5 in [9], Chapters 9 and 10 in [1], or Chapter 8 in [12]. Therefore, δ is often small for x such that $x < n$ and $J_\nu(x) = 0$.

The following theorem states a simple Sturm sequence property of the eigenvalues of tridiagonal matrices whose entries on the sub- and super-diagonals are positive.

Theorem 21 *Suppose that n is a positive integer and T is a tridiagonal real $n \times n$ matrix such that all entries on the sub- and super-diagonals of T are positive.*

Then, every eigenvalue of T is simple/non-degenerate.

Proof. Theorem 1 in Section 1 of Chapter II in [2] provides a slightly more general formulation of the present theorem. \square

The following corollary states a simple Sturm sequence property of the eigenvalues of T defined in (38).

Corollary 22 *Suppose that ν is a nonnegative real number and n is a positive integer.*

Then, every eigenvalue of T defined in (38) is simple/non-degenerate.

Proof. Theorem 21 yields the present corollary. \square

The following lemma bounds the distance between an approximate eigenvalue and the actual eigenvalue nearest to the approximation.

Lemma 23 *Suppose that λ and μ are real numbers, n is a positive integer, T is a real self-adjoint $n \times n$ matrix, and v is a real $n \times 1$ column vector such that λ is the eigenvalue of T nearest to μ , and*

$$\sum_{k=1}^n (v_k)^2 = 1. \quad (44)$$

Then,

$$|\mu - \lambda| \leq \sqrt{2} \sqrt{\sum_{k=1}^n \left((T v)_k - \mu v_k \right)^2}, \quad (45)$$

where $(T v)_1, (T v)_2, \dots, (T v)_{n-1}, (T v)_n$ are the entries of the matrix-vector product $T v$.

Proof. Theorem 8.1.13 in [3] provides a somewhat more general formulation of the present lemma. \square

The following lemma bounds the changes in the eigenvalues and eigenvectors induced by using the truncated matrix T defined in (38) (which is only $n \times n$ rather than infinite-dimensional).

Lemma 24 *Suppose that λ, μ, ν , and x are real numbers, n is a positive integer, and u is a real $n \times 1$ column vector such that $\nu \geq 0$, $x > 0$, (43) holds, λ is the eigenvalue of T nearest to $\frac{1}{x}$, μ is the eigenvalue of T nearest but not equal to λ ,*

$$T u = \lambda u, \quad (46)$$

and

$$\sum_{k=1}^n (u_k)^2 = 1, \quad (47)$$

where T is defined in (38).

Then,

$$\left| \frac{1}{x} - \lambda \right| \leq \sqrt{2} \delta, \quad (48)$$

and either (or both)

$$|v_k - u_k| \leq \frac{4\sqrt{n} \delta}{|\mu - \lambda|} \quad (49)$$

for $k = 1, 2, \dots, n-1, n$, or

$$|-v_k - u_k| \leq \frac{4\sqrt{n} \delta}{|\mu - \lambda|} \quad (50)$$

for $k = 1, 2, \dots, n-1, n$, where $v = v(x)$ is defined in (39) and $\delta = \delta(x)$ is defined in (40).

Proof. Combining (45), (41), and (42) yields (48).

For any real $n \times 1$ column vector a , we define

$$\|a\| = \sqrt{\sum_{k=1}^n (a_k)^2}. \quad (51)$$

Due to (47),

$$\|u\| = 1, \quad (52)$$

and, due to (39),

$$\|v\| = 1. \quad (53)$$

Defining

$$c = \sum_{k=1}^n u_k v_k \quad (54)$$

and

$$w = v - c u, \quad (55)$$

we observe that cu is the component of v along u and that w is the projection of v onto the orthogonal complement of the space spanned by u , so that u and w are orthogonal, that is,

$$\sum_{k=1}^n u_k w_k = 0 \quad (56)$$

(we can also obtain (56) by substituting (55) into the left hand side of (56) and using (52) and (54) to simplify the result). Combining (55), (56), (52), and (53) yields that

$$1 = \|v\|^2 = c^2 + \|w\|^2 \quad (57)$$

and

$$\|\operatorname{sgn}(c)v - u\|^2 = (|c| - 1)^2 + \|w\|^2, \quad (58)$$

where

$$\operatorname{sgn}(c) = \begin{cases} 1, & c > 0 \\ -1, & c < 0 \\ 0, & c = 0. \end{cases} \quad (59)$$

Combining (57) and (58) yields that

$$\|\operatorname{sgn}(c)v - u\|^2 = 2(1 - |c|). \quad (60)$$

Due to (57),

$$1 - |c| = \frac{\|w\|^2}{1 + |c|}. \quad (61)$$

Combining (60) and (61) yields that

$$\|\operatorname{sgn}(c)v - u\|^2 \leq 2\|w\|^2. \quad (62)$$

Moreover,

$$\|w\| \leq \|(T - \lambda \mathbf{1})^{-1}\| \|(T - \lambda \mathbf{1})w\|, \quad (63)$$

where $\mathbf{1}$ is the diagonal $n \times n$ identity matrix with the entry

$$\mathbf{1}_{j,k} = \begin{cases} 1, & j = k \\ 0, & j \neq k \end{cases} \quad (64)$$

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

$$\|(T - \lambda \mathbf{1})^{-1}\| = \sup_{a \in \mathbb{R}^n: \|a\| \neq 0} \frac{\|(T - \lambda \mathbf{1})^{-1}a\|}{\|a\|}. \quad (65)$$

Combining (55) and (46) yields that

$$(T - \lambda \mathbf{1})w = (T - \lambda \mathbf{1})v. \quad (66)$$

Furthermore,

$$\|(T - \lambda \mathbf{1})v\| \leq \left\|Tv - \frac{1}{x}v\right\| + \left\|\left(\frac{1}{x} - \lambda\right)v\right\|. \quad (67)$$

Due to (41) and (42),

$$\left\| T v - \frac{1}{x} v \right\| \leq \delta. \quad (68)$$

Combining (48) and (53) yields that

$$\left\| \left(\frac{1}{x} - \lambda \right) v \right\| \leq \sqrt{2} \delta. \quad (69)$$

Combining (63), (66), (67), (68), and (69) yields that

$$\|w\| \leq (1 + \sqrt{2}) \delta \|(T - \lambda \mathbf{1})^{-1}\|. \quad (70)$$

Since T is self-adjoint, all eigenvalues of T are real; therefore, keeping in mind Corollary 22,

$$\|(T - \lambda \mathbf{1})^{-1}\| = \frac{1}{|\mu - \lambda|}. \quad (71)$$

Combining (62), (70), and (71) yields that (49) holds for $k = 1, 2, \dots, n-1, n$, or that (50) holds for $k = 1, 2, \dots, n-1, n$. \square

Suppose that ν is a nonnegative real number and n is a positive integer. We define x_1, x_2, x_3, \dots to be all of the positive real numbers such that

$$J_\nu(x_k) = 0 \quad (72)$$

for any positive integer k , ordered so that

$$0 < x_1 < x_2 < x_3 < \dots, \quad (73)$$

where J_ν is the Bessel function of the first kind of order ν (see, for example, [12]). We define S to be the diagonal real $n \times n$ matrix with the entry

$$S_{j,k} = \begin{cases} \sqrt{\sum_{m=1}^n (f_m(x_j))^2}, & j = k \\ 0, & j \neq k \end{cases} \quad (74)$$

for $j, k = 1, 2, \dots, n-1, n$, where $f_1, f_2, \dots, f_{n-1}, f_n$ are defined in (34), and $x_1, x_2, \dots, x_{n-1}, x_n$ are defined in (72) and (73). We define e to be the real $n \times 1$ column vector with the entry

$$e_k = \begin{cases} 1, & k = 1 \\ 0, & k \neq 1 \end{cases} \quad (75)$$

for $k = 1, 2, \dots, n-1, n$.

The following lemma expresses in matrix notation the evaluations of linear combinations of Bessel functions for which Subsection 3.4 describes fast algorithms.

Lemma 25 *Suppose that ν is a nonnegative real number, n is a positive integer, and α and β are real $n \times 1$ column vectors such that α has the entry*

$$\alpha_j = \sum_{k=1}^n \beta_k f_k(x_j) \quad (76)$$

for $j = 1, 2, \dots, n-1, n$, where $f_1, f_2, \dots, f_{n-1}, f_n$ are defined in (34), and $x_1, x_2, \dots, x_{n-1}, x_n$ are defined in (72) and (73).

Then,

$$|\alpha_k - (S U^T \beta)_k| \leq \frac{4 S_{k,k} \sqrt{n} \delta(x_k)}{|\mu_k - \lambda_k|} \quad (77)$$

for any $k = 1, 2, \dots, n-1, n$ such that

$$\frac{4 S_{k,k} \sqrt{n} \delta(x_k)}{|\mu_k - \lambda_k|} < |f_1(x_k)|, \quad (78)$$

where λ_k is the eigenvalue of T defined in (38) nearest to $\frac{1}{x_k}$, μ_k is the eigenvalue of T nearest but not equal to λ_k , $\delta = \delta(x_k)$ is defined in (40), U is a real $n \times n$ matrix whose k^{th} column is the normalized eigenvector of T corresponding to the eigenvalue λ_k whose first entry has the same sign as $f_1(x_k)$, S is defined in (74), and $(S U^T \beta)_k$ is the k^{th} entry of the matrix-matrix-vector product $S U^T \beta$.

Proof. Combining (49), (39), and (74) yields (77); (78) simply guarantees that (49) holds rather than (50). \square

The following two lemmas provide alternative expressions for the entries of S defined in (74).

Lemma 26 *Suppose that ν is a nonnegative real number and n is a positive integer.*

Then,

$$\left| S_{k,k} - \frac{f_1(x_k)}{(U^T e)_k} \right| \leq \frac{4 S_{k,k} \sqrt{n} \delta(x_k)}{|\mu_k - \lambda_k| |(U^T e)_k|} \quad (79)$$

for any $k = 1, 2, \dots, n-1, n$ such that (78) holds, where S is defined in (74), f_1 is defined in (34), $x_1, x_2, \dots, x_{n-1}, x_n$ are defined in (72) and (73), λ_k is the eigenvalue of T defined in (38) nearest to $\frac{1}{x_k}$, μ_k is the eigenvalue of T nearest but not equal to λ_k , $\delta = \delta(x_k)$ is defined in (40), U is a real $n \times n$ matrix whose k^{th} column is the normalized eigenvector of T corresponding to the eigenvalue λ_k whose first entry has the same sign as $f_1(x_k)$, e is defined in (75), and $(U^T e)_k$ is the k^{th} entry of the matrix-vector product $U^T e$.

Proof. Combining (49), (39), and (75) yields that

$$\left| (U^T e)_k - \frac{f_1(x_k)}{\sqrt{\sum_{m=1}^n (f_m(x_k))^2}} \right| \leq \frac{4 \sqrt{n} \delta(x_k)}{|\mu_k - \lambda_k|} \quad (80)$$

for any $k = 1, 2, \dots, n-1, n$ such that (78) holds; as in the proof of (77), (78) guarantees that (49) holds rather than (50). Combining (74) and (80) yields (79). \square

Lemma 27 *Suppose that ν is a nonnegative real number and n is a positive integer.*

Then,

$$f_1(x_k) = -\frac{2^\nu \Gamma(\nu + 1) \sqrt{\nu + 1}}{(x_k)^\nu} \frac{d}{dx} J_\nu(x_k) \quad (81)$$

for $k = 1, 2, \dots, n-1, n$, where f_1 is defined in (34), $x_1, x_2, \dots, x_{n-1}, x_n$ are defined in (72) and (73), Γ is the gamma (factorial) function, and J_ν is the Bessel function of the first kind of order ν (see, for example, [12]).

Proof. Formula 4 of Section 3.2 in [12] provides a somewhat more general formulation of (81). \square

Remark 28 The right hand side of (79) involves the potentially troublesome quantity

$$\frac{1}{|(U^T e)_k|}. \quad (82)$$

However, due to (49), (39), and (74), if the quantity

$$\frac{4\sqrt{n}\delta(x_k)}{|\mu_k - \lambda_k|} \quad (83)$$

is small, then (82) is accordingly close to the quantity

$$\frac{S_{k,k}}{|f_1(x_k)|}, \quad (84)$$

which should not be unreasonably large.

Remark 29 Numerical experiments indicate that the quantity $|\mu_k - \lambda_k|$ in (77) and (79) is never exceedingly small for practical ranges of n ; this is probably fairly easy to prove, perhaps using the properties of Sturm sequences. The following remark might help.

Remark 30 Suppose that $\nu = 0$ and n is a positive integer. For any positive real number x , we define $\tilde{v} = \tilde{v}(x)$ to be the real $n \times 1$ column vector with the entry

$$\tilde{v}_k = (-1)^k v_k \quad (85)$$

for $k = 1, 2, \dots, n-1, n$, where $v = v(x)$ is defined in (39). Then, Formula 1 of Section 3.2 in [12] and Formula 2 of Section 2.1 in [12] lead to

$$\left| (T \tilde{v})_n + \frac{1}{x} \tilde{v}_n \right| \leq \delta \quad (86)$$

in place of (41),

$$(T \tilde{v})_k = -\frac{1}{x} \tilde{v}_k \quad (87)$$

for $k = 1, 2, \dots, n-2, n-1$ in place of (42), etc.

The following lemma states a special case of the Gegenbauer addition formula for Bessel functions.

Lemma 31 *Suppose that $\nu = \frac{1}{2}$.*

Then,

$$\sum_{m=0}^{\infty} (f_m(x))^2 = \frac{1}{2} \quad (88)$$

for any positive real number x , where f_0, f_1, f_2, \dots are defined in (34).

Proof. Formula 3 of Section 11.4 in [12] provides a somewhat more general formulation of (88). \square

The following lemma provides alternative expressions for the entries of S defined in (74) for what are known as spherical Bessel functions of the first kind.

Lemma 32 *Suppose that $\nu = \frac{1}{2}$, ε is a positive real number, and k and n are positive integers such that*

$$\sum_{m=n+1}^{\infty} (f_m(x_k))^2 \leq \varepsilon, \quad (89)$$

where $f_{n+1}, f_{n+2}, f_{n+3}, \dots$ are defined in (34), and x_k is defined in (72) and (73).

Then,

$$\left| (S_{k,k})^2 - \frac{1}{2} \right| \leq \varepsilon, \quad (90)$$

where $S_{k,k}$ is defined in (74).

Proof. Combining (74), (88), (89), and (72) yields (90). \square

Remark 33 As in Remark 20, it is often possible to have ε in (89) and (90) be small for k such that $x_k < n$.

3 Fast algorithms

Each subsection in the present section relies on both Subsection 2.1 and either Subsection 2.2 or Subsection 2.3. We describe the algorithms in Subsections 3.1 and 3.2 solely to illustrate the generality of the techniques discussed in the present paper; we would expect specialized schemes to outperform the algorithms described in Subsections 3.1 and 3.2 in most, if not all, practical circumstances.

3.1 Quadrature nodes and Christoffel numbers associated with orthonormal polynomials

The entries of Λ in (19) are the nodes $x_0, x_1, \dots, x_{n-2}, x_{n-1}$ in (28). We can compute rapidly the entries of Λ in (19) using algorithm A_1 from Remark 1, due to (19), since T in (19) is tridiagonal, real, and self-adjoint, U in (19) is real and unitary, and Λ in (19) is diagonal, with diagonal entries that according to (12) are distinct. For the same reason, we can apply rapidly the matrix U^T to the vector e in (24) using algorithm A_3 from Remark 1. We can then compute the Christoffel numbers $w_0, w_1, \dots, w_{n-2}, w_{n-1}$ in (28) using (29) and (24).

3.2 Zeros of Bessel functions

We can compute rapidly the zeros $x_1, x_2, \dots, x_{n-1}, x_n$ defined in (72) and (73) for which δ defined in (40) is sufficiently small, using (48) and algorithm A_1 from Remark 1, since T defined in (38) is tridiagonal, real, and self-adjoint, and (according to Corollary 22) has n distinct eigenvalues.

3.3 Decompositions into and reconstructions from linear combinations of weighted orthonormal polynomials

We can apply rapidly the matrices U and U^T in (23) and (22) using algorithms A_2 and A_3 from Remark 1, due to (19), since T in (19) is tridiagonal, real, and self-adjoint, U in (19) is real and unitary, and Λ in (19) is diagonal, with diagonal entries that according to (12) are distinct. Furthermore, we can apply rapidly the remaining matrices S and S^{-1} in (22) and (23), since S and S^{-1} in (22) and (23) are diagonal, once we use (29) and the algorithms from Subsection 3.1 to compute the entries of S and S^{-1} .

Remark 34 We can construct fast algorithms for decomposing into and reconstructing from linear combinations of associated Legendre functions using the algorithms described in the present subsection. For any nonnegative integers l and m , the normalized associated Legendre function of order m and degree l (often denoted by \overline{P}_l^m) is equal to the function q_{l-m} defined in (14) for the orthonormal polynomials on $[-1, 1]$ for the weight w defined by

$$w(x) = (1 - x)^m (1 + x)^m. \quad (91)$$

Hence, we could utilize the algorithms discussed in the present subsection exactly as described. However, to take advantage of the symmetries of associated Legendre functions, we would want to diagonalize the square T^2 of the matrix T in (19) rather than T itself, modifying the algorithms from Remark 1 appropriately, for increased efficiency. We might also want to compute interpolations to and from values at the zeros of various polynomials, using the Christoffel-Darboux formula, as first introduced in [7] and [13], and subsequently optimized. For details on the connections between associated Legendre functions and spherical harmonics, see, for example, [10].

3.4 Evaluations of linear combinations of Bessel functions

We can apply rapidly the matrix U^T in (77) using algorithm A_3 from Remark 1, since T defined in (38) is tridiagonal, real, and self-adjoint, and (according to Corollary 22) has n distinct eigenvalues, and hence U in (77) can be chosen to be real and unitary. Furthermore, we can apply rapidly the remaining matrix S in (77), since S in (77) is diagonal, once we use (79), algorithm A_3 from Remark 1, and the algorithm from Subsection 3.2 to compute the entries of S .

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