The Application of the Fast Fourier Transform to Jacobi Polynomial expansions

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Abstract

We observe that the exact connection coefficient relations transforming modal coefficients of one Jacobi Polynomial class to the modal coefficients of certain other classes are sparse. Because of this, when one of the classes corresponds to the Chebyshev case, the Fast Fourier Transform can be used to quickly compute modal coefficients for Jacobi Polynomial expansions of class (α, β) when 2α and 2β are both odd integers. In addition, we present an algorithm for computing Jacobi spectral expansions that is more robust than Jacobi-Gauss quadrature. Numerical results are presented that illustrate the computational efficiency and accuracy advantage of our method over standard quadrature methods.

1 Introduction

The classical Jacobi Polynomials $P_n^{(\alpha,\beta)}$ are a family of orthogonal polynomials [22] that have been used extensively in many applications for their ability to approximate general classes of functions. They are a class of polynomials that encompass the Chebyshev, Legendre, and Gegenbauer/ultraspheric polynomials. In addition, they have a very close connection to the Associated Legendre functions that are widely used in Spherical Harmonic expansions.

Jacobi polynomial expansions have been used in a variety of applications, some of which are the resolution of the Gibbs' phenomenon [14], electrocardiogram data compression [23], and the solution to differential equations [8]. Due to the range of applications for Jacobi polynomials, it is desirable to perform spectral expansion computations as quickly and accurately as possible. In this paper, we show that for a variety of (but not all) classes of Jacobi polynomials, one can exploit the Fast Fourier Transform (FFT) to perform spectral transformations; this implies an asymptotic reduction of the direct-method unoptimized $O(N^2)$ cost to an $O(N \log N)$ cost, which is significant if N is large. In addition, we show that computational savings is apparent even for small N. Our method is applicable for discrete polynomial transforms for an expansion in $\left\{P_n^{(\alpha,\beta)}\right\}_{n=0}^{N-1}$ if both 2α and 2β are odd integers. This notably does not include the Legendre case where $(\alpha, \beta) = (0, 0)$.

The idea of using an FFT to compute Jacobi spectral transformations is not new. That the FFT can be used to compute Chebyshev modes via nodal evaulations at the Chebyshev quadrature points is well-known [16]. In addition, using the FFT for other Jacobi polynomial transformations has been studied. For Legendre polynomial transforms, Alpert [2] employed a submatrix decomposition of the modal connection matrix to travel between Chebyshev modes and Legendre modes. Orszag [19] used the WKB approximation to propose an algorithm for a broad class of eigenfunction transforms (including Legendre polynomial transforms). Driscoll [9], [10] provides an $O(N \log N)$ algorithm for general discrete polynomial transforms as long as the three-term recurrence for the polynomial family is known. The method relies in part on a Toeplitz-product factorization of the interpolating Vandermonde matrix, for which an asymptotic $O(N \log N)$ algorithm for matrix-vector multiplication exists [20].

Our method is based upon two main observations: firstly that the transformation from function evaluations located at the Chebyshev quadrature nodes to Chebyshev polynomial expansion coefficients can be implemented with the FFT. Secondly, we show that the exact connection coefficient relation between Chebyshev polynomials and several other Jacobi polynomials classes can be computed and implemented robustly in an inexpensive $O(N)$ cost. The connection coefficient relation is simple enough that it does not require the evaluation of any transcendental or higher-order functions, requires very little preprocessing, and only $O(N)$ storage is required. This should be compared to the previously mentioned methods which are either approximate in the computation, require more preprocessing, more storage, and/or are significantly more complicated to implement. The disadvantage of our method is that it can only be applied for certain classes of Jacobi Polynomials that, as already mentioned, excludes the Legendre case.

In section 2 we give an overview of Jacobi polynomials and the relevant properties needed for our discussion. Section 3 is devoted to a theoretical description of the method and includes most of the major results. Section 4 is a special application of the results from section 3 to Chebyshev-like systems where the FFT may be exploited. Finally, section 5 gives some numerical examples.

2 Jacobi Polynomials

For a comprehensive treatement of Jacobi polynomials and their properties, [22], [11], and [1] prove to be excellent references. All properties and results that follow in this section are taken from these references. Jacobi polynomials are one of the two linearly independent solutions to the linear, second-order, singular Sturm-Liouville differential equation

$$-\frac{\mathrm{d}}{\mathrm{d}r}\left[(1-r)^{\alpha+1}(1+r)^{\beta+1)}\frac{\mathrm{d}\rho}{\mathrm{d}r}\right]-n(n+\alpha+\beta+1)(1-r)^{\alpha}(1+r)^{\beta}\rho=0,\qquad r\in[-1,1]. \tag{2.1}$$

The parameters α, β are restricted to take real values in the interval $(-1, \infty)$. The monic Jacobi polynomial of order n, as a solution to (2.1), is written as $P_n^{(\alpha,\beta)}(r)$. We define the dimension-N space $\mathcal{B}_N = \mathrm{span}\{r^n : 0 \le n \le N-1\}$. For any $\alpha, \beta > -1$, the Jacobi polynomials of class (α, β) are orthogonal under a weighted L^2 inner product:

$$\int_{-1}^{1} P_m^{(\alpha,\beta)} P_n^{(\alpha,\beta)} (1-r)^{\alpha}(1+r)^{\beta}\,\mathrm{d}r = h_n^{(\alpha,\beta)}\,\delta_{m,n}, \tag{2.2}$$

where $\delta_{m,n}$ is the Kronecker delta function, and $h_n^{(\alpha,\beta)}$ is a normalization constant given in the appendix, equation (A.1). We take the integral (2.2) in the Lebesgue sense. Define the weight function

$$\omega^{(\alpha,\beta)}(r) = (1-r)^{\alpha}(1+r)^{\beta}, \tag{2.3}$$

and denote angled brackets $\langle \cdot, \cdot \rangle_{(\alpha,\beta)}$ as the inner product

$$\langle f, g \rangle_{(\alpha,\beta)} = \int_{-1}^{1} f(r)\, g(r)\, \omega^{(\alpha,\beta)}\,\mathrm{d}r.$$

This inner product induces a norm $\|\cdot\|_{(\alpha,\beta)}$ on the space $L^2_{(\alpha,\beta)} := \left\{ f : [-1,1] \to \mathbb{R} : f \text{ Lebesgue measurable}, \|f\|_{(\alpha,\beta)} < \infty \right\}$. The Jacobi polynomials of class (α, β) are complete and orthogonal in $L^2_{(\alpha,\beta)}$.

The monic Jacobi polynomials satisfy various relations and can be expressed in terms of the Hypergeometric function ${}_2F_1$, and also satisfy a generalized Rodrigues relation for all $m \leq n$:

$$\begin{pmatrix} 2n+\alpha+\beta \\ n \end{pmatrix} \omega^{(\alpha,\beta)} P_n^{(\alpha,\beta)} = \\ \frac{(-1)^m}{2^{m-n}(n-1)\cdots(n-m+1)} \frac{\mathrm{d}^m}{\mathrm{d}x^m}\Big[\omega^{(\alpha+m,\beta+m)} P_{n-m}^{(\alpha+m,\beta+m)}\Big]. \tag{2.4}$$

Although the formulae for the monic orthogonal polynomials are often easier to write down than those for other normalizations, we shall prefer to work with the $L^2_{(\alpha,\beta)}$-normalized polynomials. To this end, we define

$$\tilde{P}_n^{(\alpha,\beta)} = \frac{P_n^{(\alpha,\beta)}}{\sqrt{h_n^{(\alpha,\beta)}}},$$

which are orthonormal under the weight $\omega^{(\alpha,\beta)}$.

All orthogonal polynomials satisfy a three-term recurrence relation from which the Kernel polynomials and the Christoffel-Darboux identity can be derived. These last two properties yield the following *promotions* and *demotions* of the Jacobi polynomial class parameters (α, β):

$$(1-r)\,\tilde{P}_n^{(\alpha,\beta)} = \mu_{n,0}^{(\alpha,\beta)}\,\tilde{P}_n^{(\alpha-1,\beta)} - \mu_{n,1}^{(\alpha,\beta)}\tilde{P}_{n+1}^{(\alpha-1,\beta)}, \tag{2.5}$$

$$(1+r)\tilde{P}_n^{(\alpha,\beta)} = \mu_{n,0}^{(\beta,\alpha)}\,\tilde{P}_n^{(\alpha,\beta-1)} + \mu_{n,1}^{(\beta,\alpha)}\tilde{P}_{n+1}^{(\alpha,\beta-1)}, \tag{2.6}$$

$$\tilde{P}_n^{(\alpha,\beta)} = \nu_{n,0}^{(\alpha,\beta)}\tilde{P}_n^{(\alpha+1,\beta)} - \nu_{n,-1}^{(\alpha,\beta)}\tilde{P}_{n-1}^{(\alpha+1,\beta)}, \tag{2.7}$$

$$\tilde{P}_n^{(\alpha,\beta)} = \nu_{n,0}^{(\beta,\alpha)}\tilde{P}_n^{(\alpha,\beta+1)} + \nu_{n,-1}^{(\beta,\alpha)}\tilde{P}_{n-1}^{(\alpha,\beta+1)}, \tag{2.8}$$

where $\mu_{n,0/1}^{(\alpha,\beta)}$ and $\nu_{n,0/-1}^{(\alpha,\beta)}$ are constants for which we derive explicit formulae in appendix A. The formulae (2.5)-(2.8) are the main ingredients for our results.

Lastly we cover the spectral expansion of a function $f(r)$ in Jacobi polynomials. For any $f \in L^2_{(\alpha,\beta)}$ we define the modal coefficients

$$\hat{f}_n^{(\alpha,\beta)} = \Big\langle f, \tilde{P}_n^{(\alpha,\beta)} \Big\rangle_{(\alpha,\beta)}.$$

We also have a Parseval-type relation:

$$\|f\|^2_{(\alpha,\beta)} = \sum_{n=0}^{\infty} \Big[\,\hat{f}_n^{(\alpha,\beta)}\Big]^2.$$

Naturally, $\hat{f}_n^{(a,b)}$ is well-defined if $a \geq \alpha$ and $b \geq \beta$ because of the inclusion $L^2_{(\alpha,\beta)} \subseteq L^2_{(a,b)}$. We define the projection operator

$$\mathcal{P}_N^{(\alpha,\beta)} f = \sum_{n=0}^{N-1} \hat{f}_n^{(\alpha,\beta)}\,\tilde{P}_n^{(\alpha,\beta)}.$$

By completeness and orthogonality, this operator satisfies the relations

$$\left\| f - \mathcal{P}_n^{(\alpha,\beta)} f \right\|_{(\alpha,\beta)} \longrightarrow 0, \qquad n \to \infty$$

$$\left\langle f - \mathcal{P}_n^{(\alpha,\beta)} f, \phi \right\rangle_{(\alpha,\beta)} = 0, \qquad \phi \in \mathcal{B}_n$$

2.1 Connection Coefficients

The problem of rewriting an expansion of one class of Jacobi polynomials into an expansion in a different class can be cast as the problem of determining the connection coefficients $\lambda_{n,m}^{(\alpha,\beta,\gamma,\delta)}$ satisfying

$$\tilde{P}_n^{(\alpha,\beta)} = \sum_{m=0}^{n} \lambda_{n,m}^{(\alpha,\beta,\gamma,\delta)} \tilde{P}_m^{(\gamma,\delta)}. \tag{2.9}$$

We clearly have by orthogonality that

$$\lambda_{n,m}^{(\alpha,\beta,\gamma,\delta)} = \left\langle \tilde{P}_n^{(\alpha,\beta)}, \tilde{P}_m^{(\gamma,\delta)} \right\rangle_{(\gamma,\delta)} \tag{2.10}$$

These connection coefficients are explicitly known for a very large class of problems. Askey [4] compiles earlier formulae originated by Gegenbauer to give explicit formulae for the $\lambda_{m,n}^{(\alpha,\beta,\gamma,\delta)}$ for the different cases (a) $\alpha = \gamma$, (b) $\beta = \delta$, and (c) $\alpha = \beta$ and $\gamma = \delta$. These relations can in general be bootstrapped to determine the general coefficients for any (α, β, γ, δ). In terms of the hypergeometric function ${}_3F_2$, an explicit expression for the connection coefficients can also been derived from the Rodrigues relation (2.4). See e.g. [3].

An alternative expression has been derived by Maroni and da Rocha [17] utilizing a recurrence relation satisfied by the connection coefficients in conjunction with significant symbolic computational arithmetic. The disadvantage of both of these methods is that the computation of these connection coefficients requires a relatively sophisticated algorithm. Askey's method does not actually give the connection coefficients explicitly if α is different from γ and β is different from δ, and the coefficients that are given require the computation of falling factorials and possibly Gamma functions; of course one may evaluate the function ${}_3F_2$, but that is likewise relatively complicated. Maroni's results give explicit formulae for the λ coefficients, but require the computation of several products and sums of Gamma functions for each coefficient.

Even if the coefficients λ can be computed quickly and accurately, in order to transfer modal coefficients of class (α, β) into those of class (γ, δ), the sum

$$\hat{f}_n^{(\gamma,\delta)} = \sum_{m=n}^{\infty} \lambda_{m,n}^{(\gamma,\delta,\alpha,\beta)} \hat{f}_m^{(\alpha,\beta)} \tag{2.11}$$

must be computed in some fashion if the *exact* modes $\hat{f}_n^{(\gamma,\delta)}$ are desired. If we wish to simply approximate the modes, we may assume that $\hat{f}_m^{(\alpha,\beta)} = 0$ for $m > N$ for some large N. In this case, we still must perform the operation (2.11) (with the upper limit truncated to N) for each $n = 0, 1, 2, ..., N-1$, which takes $O(N^2)$ operations as written.

The main contribution of this paper to the problem of finding connection coefficients is given in section 3. We will assume certain restrictions on the values of α, β, γ, and δ and show that the infinite sum (2.11) is actually a finite sum (independent of the truncation order N) allowing us in theory to *exactly* compute the modes $\hat{f}_n^{(\gamma,\delta)}$ from a finite collection of modes $\hat{f}_n^{(\alpha,\beta)}$, and the computation of each mode can be done in an operation count that is n-independent. In practice, we must still compute the connection coefficients $\lambda_{m,n}^{(\gamma,\delta,\alpha,\beta)}$. While e.g. Askey's or Maroni's formulae may in principle be used to accomplish this, we also present a simple algorithm for robustly computing the connection coefficients assuming restrictions (to be given in the next section) on the quartet $(\alpha, \beta, \gamma, \delta)$.

3 Jacobi-Jacobi transformations

The purpose of this section is to form a relationship between the expansions $\mathcal{P}_N^{(\alpha,\beta)} f$ and $\mathcal{P}_N^{(\gamma,\delta)} f$ for $\alpha \neq \gamma$ and/or $\beta \neq \delta$. More than that, we will determine a relationship that will allow us to travel between the two expansions robustly and with very little effort. Of course, the speed of this transformation comes with a natural price: this can only be done when $|\delta - \beta|$ and $|\gamma - \alpha|$ are integers.

We begin by proving a lemma that is an inductive application of equations (2.5) and (2.6):

Lemma 3.1.
For any $A, B \in \mathbb{N}$ and $\alpha, \beta > -1$, the following promotion relations hold:

$$(1-r)^A \tilde{P}_n^{(\alpha+A,\beta)} = \sum_{m=0}^{A} M_{m,n}^{(\alpha,A,\beta)} \tilde{P}_{n+m}^{(\alpha,\beta)} \tag{3.1}$$

$$(1+r)^B \tilde{P}_n^{(\alpha,\beta+B)} = \sum_{m=0}^{B} (-1)^m M_{m,n}^{(\beta,B,\alpha)} \tilde{P}_{n+m}^{(\alpha,\beta)}, \tag{3.2}$$

where the $M_{m,n}^{(\alpha,\beta)}$ are constants. Similarly, we can demote the class parameters $\alpha + A$ and $\beta + B$ down to α and β as well:

$$\tilde{P}_n^{(\alpha,\beta)} = \sum_{m=0}^{A} N_{m,n}^{(\alpha,A,\beta)} \tilde{P}_{n-m}^{(\alpha+A,\beta)} \tag{3.3}$$

$$\tilde{P}_n^{(\alpha,\beta)} = \sum_{m=0}^{B} (-1)^m N_{m,n}^{(\beta,B,\alpha)} \tilde{P}_{n-m}^{(\alpha,\beta+B)} \tag{3.4}$$

Proof. The proofs of (3.1) and (3.2) are accomplished via the demotion relations (2.5) and (2.6): repeated application of (2.5) to the left-hand side of (3.1), and repeated application of (2.6) to the left-hand side of (3.2) yields the desired result.

The relations (3.3) and (3.4) are proven in exactly the same fashion using the promotion relations (2.7) and (2.8). □

Note that we did not give the formulae for the constants $M_{m,n}^{(\alpha,A,\beta)}$ and $N_{m,n}^{(\alpha,A,\beta)}$ in Lemma 3.1. It would be possible for us to derive such formulae in terms of the $\mu_{n,i}^{(\alpha,\beta)}$ and $\nu_{n,i}^{(\alpha,\beta)}$, but it is of little value. The main use of Lemma 3.1 is in the proof of the following theorem:

Theorem 3.2.
For $A, B \in \mathbb{N}_0$ and $\alpha, \beta > -1$, let $f \in L^2_{(\alpha,\beta)}$. Then

$$\hat{f}_n^{(\alpha+A,\beta+B)} = \sum_{m=0}^{A+B} \lambda_{n+m,n}^{(\alpha+A,\beta+B,\alpha,\beta)} \hat{f}_{n+m}^{(\alpha,\beta)}, \qquad n \geq 0 \tag{3.5}$$

where the $\lambda_{n+m,n}^{(\alpha+A,\beta+B,\alpha,\beta)}$ are the connection coefficients (2.10).

Proof. For ease of exposition, we drop the superscripts on $\lambda_{n+m,n}^{(\alpha+A,\beta+B,\alpha,\beta)}$ in this proof. We use Lemma 3.1 twice on $(1-r)^A(1+r)^B \tilde{P}_n^{(\alpha+A,\beta+B)}$ to show that there exist constants $\Lambda_{n+m,n}$ such that

$$\omega^{(A,B)} \tilde{P}_n^{(\alpha+A,\beta+B)} = \sum_{m=0}^{A+B} \Lambda_{n+m,n} \tilde{P}_{n+m}^{(\alpha,\beta)}.$$

Following this we note that $\hat{f}_n^{(\alpha,\beta)}$ is well-defined because $f \in L^2_{(\alpha,\beta)}$, and $\hat{f}_n^{(\alpha+A,\beta+B)}$ is well-defined because of the inclusion of $L^2_{(\alpha,\beta)}$ in $L^2_{(\alpha+A,\beta+B)}$. Finally, we have

$$\begin{aligned}
\hat{f}_n^{(\alpha+A,\beta+B)} &= \left\langle f, \tilde{P}_n^{(\alpha+A,\beta+B)} \right\rangle_{(\alpha+A,\beta+B)} \\
&= \left\langle f, (1-r)^A (1+r)^B \tilde{P}_n^{(\alpha+A,\beta+B)} \right\rangle_{(\alpha,\beta)} \\
&= \left\langle f, \sum_{m=0}^{A+B} \Lambda_{n+m,n} \tilde{P}_{n+m}^{(\alpha,\beta)} \right\rangle_{(\alpha,\beta)} \\
&= \sum_{m=0}^{A+B} \Lambda_{n+m,n} \left\langle f, \tilde{P}_{n+m}^{(\alpha,\beta)} \right\rangle_{(\alpha,\beta)} \\
&= \sum_{m=0}^{A+B} \Lambda_{n+m,n} \hat{f}_{n+m}^{(\alpha,\beta)}.
\end{aligned}$$

Furthermore, it is easy to show by orthogonality that $\Lambda_{n+m,n} \equiv \lambda_{n+m,n}$, where $\lambda_{n+m,n}$ are the Jacobi connection coefficients (2.10). □

Remark 3.3. Theorem 3.2 may also be proven by utilizing equations (2.7)-(2.8) and by noting that the projection operator $\mathcal{P}_N^{(\alpha,\beta)}$ is the identity operator on the space of $(N-1)^{\text{st}}$ degree polynomials $\mathcal{B}_N$ for any pair (α,β). In this case it is trivial to see that $\Lambda_{n+m,n} \equiv \lambda_{n+m,n}$.

Theorem 3.2 gives us a special version of the connection coefficient relation (2.11). In the language of section 2.1, we have derived a result when $\gamma = \alpha + A$ and $\delta = \beta + B$. It says that we can express the modes of higher-class Jacobi expansions in terms of a *finite* linear combinations of lower-class Jacobi expansions. This relation is exact. Roughly speaking, in order to convert an expansion of class (α,β) to one of class $(\alpha+A,\beta+B)$, we require about $O(A+B)$ computations, as long as A and B are both natural numbers.

The above result is likely known by many authors in this field due to the voluminous literature on Jacobi polynomials. In particular, the connection coefficient relations presented by e.g. Askey [4] and Maroni [17] can no doubt be simplified with the assumptions of Theorem 3.2 to produce the result. However we have not seen this observation made in the literature, and so we present the above theorem.

One deficiency in the theorem above is that we do not present explicit values of the connection coefficients $\Lambda_{m,n}^{(A,B,\alpha,\beta)}$. While this is a notable loss (especially since in principle such formulae, albeit cumbersome, are present in existing literature), it is of little consequence as we present a rather straightforward algorithm in the next section for computing these connection coefficients. This algorithm is at worst slightly higher in operation count than if we were to derive explicit formulae. Furthermore, the numerical results in section 5 show that the one-time overhead cost we incur by computing these coefficients is insignificant compared to the savings we gain from being able to use the FFT when applicable for certain spectral mode calculations.

3.1 Computing the transformation

We collect the modes $\left\{\hat{f}_n^{(\alpha,\beta)}\right\}_{n=0}^{N+A+B-1}$ into the vector $\hat{\boldsymbol{f}}^{(\boldsymbol{\alpha},\boldsymbol{\beta})}$. Theorem 3.2 makes it clear that there exists an $N \times (N + A + B)$ connection coefficient matrix $\hat{C}$, dependent on α, β, A, and B such that

$$\hat{\boldsymbol{f}}^{(\boldsymbol{\alpha}+\boldsymbol{A},\boldsymbol{\beta}+\boldsymbol{B})} = \hat{C}\hat{\boldsymbol{f}}^{(\boldsymbol{\alpha},\boldsymbol{\beta})}. \tag{3.6}$$

(We assume that $A, B \in \mathbb{N}_0$.) This relation transports $N + A + B$ modes from an expansion in the polynomials $\tilde{P}^{(\alpha,\beta)}$ to N modes from an expansion in $\tilde{P}^{(\alpha+A,\beta+B)}$. The entries of the matrix $\hat{C}$ are the connection coefficients $\hat{C}_{m,n} = \lambda_{n,m}^{(\alpha+A,\beta+B,\alpha,\beta)}$, but we only have relatively complicated expressions for the explicit entries of the matrix $\hat{C}$ (see e.g. [4], [17]). In order to more easily construct the matrix $\hat{C}$ we first note that it is a sparse matrix, banded upper-triangular, with about $(A+B)(N+A+B)$ non-zero entries. To construct $\hat{C}$, we essentially write out the proof of Lemma 3.1 via induction. To this end, let us define the following set of matrices: let $U^{(\alpha,\beta)}$ and $V^{(\alpha,\beta)}$ be bidiagonal matrices with entries defined by

$$\left.\begin{aligned} U_{n,n}^{(\alpha,\beta)} &= \mu_{n,0}^{(\alpha,\beta)} \\ U_{n,n+1}^{(\alpha,\beta)} &= -\mu_{n,1}^{(\alpha,\beta)} \\ V_{n,n}^{(\alpha,\beta)} &= \mu_{n,0}^{(\beta,\alpha)} \\ V_{n,n+1}^{(\alpha,\beta)} &= -\mu_{n,1}^{(\beta,\alpha)} \end{aligned}\right\} \qquad n = 1, 2, ..., N+A+B-1$$

$$\begin{aligned} U_{N+A+B,N+A+B}^{(\alpha,\beta)} &= \mu_{n,0}^{(\alpha,\beta)} \\ V_{N+A+B,N+A+B}^{(\alpha,\beta)} &= \mu_{n,0}^{(\beta,\alpha)} \end{aligned}$$

The matrix $U^{(\alpha,\beta)}$ transforms the modes of an $(\alpha-1, \beta)$ expansion to those of an (α, β) expansion whenever $\alpha > 0$. Similarly, $V^{(\alpha,\beta)}$ transforms the modes of an $(\alpha, \beta - 1)$ expansion into those of an (α, β) expansion whenever $\beta > 0$. To define the entries of U and V we have used the demotion relations (2.5) and (2.6). Note, however, that the last mode $N + A + B$ will be incorrect because we require information about mode $N + A + B + 1$ (which we don't have) to determine it. Thus, the last output mode will be corrupted. However, given that we are merely computing connection coefficients, this 'corruption' can simply be characterized as a type of filtering of the terminal modes to reproduce the original finite-degree polynomial instead of the true set of modes $\hat{f}_n^{(\alpha+A,\beta+B)}$ for which information is embedded in the unavailable high-degree modes $\hat{f}_n^{(\alpha,\beta)}$.

We can now define a square $(N + A + B) \times (N + A + B)$ matrix C as

$$C = \prod_{b=1}^{B} V^{(\alpha+A,\beta+b)} \prod_{a=1}^{A} U^{(\alpha+a,\beta)} \tag{3.7}$$

The matrix C has some nice properties. As the product of banded bidiagonal matrices, we also know that C has non-zero entries on at most $(A + B + 1)$ diagonals, and is upper-triangular.

Proposition 3.4.

The matrix C defined by equation (3.7) is invertible and positive-definite.

Proof. C is upper-triangular, and thus the diagonal entries are the eigenvalues. By utilizing equation (3.7) and expressions (A.2) in the appendix, we have, for all $n = 1, 2, ..., N + A + B$

$$C_{n,n} \;=\; \prod_{b=1}^{B} \mu_{n,0}^{(\beta+b,\alpha+A)} \prod_{a=1}^{A} \mu_{n,0}^{(\alpha+a,\beta)} \;>\; 0 \tag{3.8}$$

□

See also e.g. [3]. Proposition 3.4 tells us that the matrix C is invertible, which means we can travel back and forth between the modes $\hat{f}_n^{(\alpha+A,\beta+B)}$ and $\hat{f}_n^{(\alpha,\beta)}$. Clearly this is the case; we did not need Proposition 3.4 to be aware of this in light of the well-posedness of the general connection coefficient problem. In practice, inverting the conventional connection coefficient problem may be difficult because of either the need to generate an additional set of connection coefficients, or because of the need to invert a full linear system. In our case, the inversion can be accomplished via back-substitution because C is banded upper-triangular. The back substitution has a sequential computational cost $O(N(A + B))$, similar to the cost of the formation or application of the matrix. Thus, promoting the parameters (α, β) by (A, B) requires a (parallelizable) $O(N)$ multiplication by C, the demotion by (A, B) requires a sequential $O(N)$ application of C^{-1}.

The positive-definiteness of C is not necessary for our results, but it hearkens to similar questions in the literature about the positivity of the Jacobi connection coefficients λ, e.g. [3]. Note however that all the entries in the matrix C are not always positive; the above proposition only deals with the main diagonal.

With the explicit expression (3.8) for the eigenvalues $C_{n,n}$, we can show that the $N \times N$ matrix C satisfies

$$\lambda_{\min}(C) \sim 2^{-(A+B)/2}, \qquad N \to \infty,$$

where $\lambda_{\min}(C)$ denotes the minimum eigenvalue of C. Since the maximum eigenvalue $C_{1,1}$ is $O(1)$, this provides a bound for the ratio between maximum and minimum eigenvalues for C. We note however that experimentally the ratio of extremal singular values of C (the condition number) seems to be much worse, and by objective standards one would judge the conditioning of C very poorly. However, we show in section 5.2 that in practice using the connection matrix is one of the more stable and robust methods available for computing modal expansions.

We tangentially note that it is not entirely necessary to form the matrix C; one can merely store the coefficients $\mu_{n,i}^{(\alpha,\beta)}$ required for the formation of C and view the application (inversion) of C as $A + B$ sequential applications (inversions) of invertible bidiagonal matrices.

Returning to the goal presented at the beginning of this section, we define the non-square matrix $\hat{C}$ as the first N rows of C, and this is exactly the matrix we were looking for. Thus, the formation of $\hat{C}$ (or C) requires $(A + B)$ multiplications between (sparse) bidiagonal matrices.

However, in contrast to the relation presented in (3.6), we prefer an invertible transformation. The reason is that we will eventually use this transform as an ingredient in a modal/nodal transformation. The matrix $\hat{C}$ is not invertible (it's not even square), but of course C is invertible, so we shall frequently use that matrix. (As mentioned before, one should be aware that the last $A + B$ modes are not the true modes, but some version of them.)

3.2 Properties of the transformation

In this section we assume that we are given a collection of modes $\left\{\hat{f}_n^{(\alpha,\beta)}\right\}_{n=0}^{\infty}$ defining a function $f=\sum_{n=0}^{\infty}\hat{f}_n^{(\alpha,\beta)}\tilde{P}_n^{(\alpha,\beta)}$, and that we wish to obtain some finite number N of the $(\alpha+A,\beta+B)$ modes. We can use the results from the previous section to compute an $N\times N$ matrix C, and an $N\times(N+A+B)$ matrix $\hat{C}$. Define the length-N vectors $\hat{\boldsymbol{f}}_{\boldsymbol{n}}^{(\mathbf{1})}$ and $\hat{\boldsymbol{f}}_{\boldsymbol{n}}^{(\mathbf{2})}$ as

$$\hat{\boldsymbol{f}}_{\boldsymbol{n}}^{(\mathbf{1})}=C\,\hat{\boldsymbol{f}}_{\boldsymbol{n}}^{(\boldsymbol{\alpha},\boldsymbol{\beta})}$$

$$\hat{\boldsymbol{f}}_{\boldsymbol{n}}^{(\mathbf{2})}=\hat{C}\hat{\boldsymbol{f}}_{\boldsymbol{n}}^{(\boldsymbol{\alpha},\boldsymbol{\beta})}.$$

The vector $\hat{\boldsymbol{f}}_{\boldsymbol{n}}^{(\boldsymbol{\alpha},\boldsymbol{\beta})}$ is of length N in the first expression, and of length $N+A+B$ in the second expression. Note that due to the definition of C (a submatrix of $\hat{C}$), we have that $\hat{f}_n^{(1)}=\hat{f}_n^{(2)}$ for $0\le n\le N-A-B-1$. Define the corresponding polynomials

$$f^{(1)}=\sum_{n=0}^{N-1}\hat{f}_n^{(1)}\,\tilde{P}_n^{(\alpha+A,\beta+B)}$$

$$f^{(2)}=\sum_{n=0}^{N-1}\hat{f}_n^{(2)}\tilde{P}_n^{(\alpha+A,\beta+B)}.$$

Application (inversion) of the matrix C is equivalent to performing the connection coefficient problem (2.11) with $\gamma=\alpha+A$ and $\delta=\beta+B$ (respectively, $\gamma=\alpha-A$, $\delta=\beta-B$). This is easy to see if one accepts the statement of remark 3.3 (namely that theorem 3.2 is just a connection coefficient problem). Therefore, it is clear that

$$f^{(1)}=\mathcal{P}_N^{(\alpha,\beta)}f.$$

Function $f^{(2)}$, the application of $\hat{C}$ is a little more subtle, but the result is that

$$f^{(2)}=\mathcal{P}_N^{(\alpha+A,\beta+B)}\mathcal{P}_{N+A+B}^{(\alpha,\beta)}f=\mathcal{P}_N^{(\alpha+A,\beta+B)}f.$$

The latter equality follows from theorem 3.2, which proves the finite termination of the modal connection expression (2.11). Therefore the two functions $f^{(1)}$ and $f^{(2)}$ are not equal; they differ in the last $A+B$ modes. Both functions can essentially be computed in the same computational time (although it does take about $\frac{1}{2}(A+B)(A+B+1)$ more operations to compute the N modes $\hat{f}_n^{(2)}$) but they are different projections. Note that the difference between these two functions is indeed important. For example in the resolution of the Gibbs' phenomenon [14] the function required is exactly the projection $\mathcal{P}^{(\alpha+A,\beta+B)}f$; the lower-order projection $\mathcal{P}^{(\alpha,\beta)}$ will not accomplish the task.

4 Exploiting the FFT

Up until this point we have not discussed any implementation issues. In this section we explore the use of the FFT for performing spectral transformations based on Jacobi polynomials. Section 4.1 introduces some necessary notation for future discussion and section 4.2 provides the methodology for using the FFT to compute Jacobi spectral expansions.

4.1 Quadrature and interpolation

All the results in this subsection are well-known and we point to the given references for details.

We shall call an N-point quadrature rule Gaussian under a particular weight function $\omega^{(\alpha,\beta)}$ if it exactly integrates any polynomial in the space $\mathcal{B}_{2N}$ under the weight $\omega^{(\alpha,\beta)}$. Such a quadrature rule always exists and is unique if the weight function is non-negative. A quadrature rule is defined by N nodes and weights $\{r_n,\, w_n\}_{n=1}^{N}$ and we shall write the Gaussian quadrature rule evaluation under weight $\omega^{(\alpha,\beta)}$ as

$$\int_{-1}^{1} f(r)\,\omega^{(\alpha,\beta)}\,\mathrm{d}r \;\simeq\; Q_N^{(\alpha,\beta)}[f] \;:=\; \sum_{n=1}^{N} f(r_n)\,w_n.$$

With this notation, we can write the definition of a Gaussian quadrature rule as one that satisfies

$$Q_N^{(\alpha,\beta)}[\phi] = \int_{-1}^{1} \phi\,\omega^{(\alpha,\beta)}\,\mathrm{d}r, \qquad\qquad \phi \in \mathcal{B}_{2N}.$$

We recall a fundamental result due to Golub and Welsch [12]: the determination of the nodes and weights $\{r_n, w_n\}$ can be accomplished via the computation of the eigenvalues and eigenvectors of a symmetric tridiagonal matrix. A more efficient way is to just compute the eigenvalues (which are the nodes r_n) and then use known formulae [5] to compute the weights w_n. This brings the cost of computation down to $O\big(N^2\big)$ operations. We refer to the nodes and weights corresponding to the Gaussian quadrature rule $Q_N^{(\alpha,\beta)}[\,\cdot\,]$ as $\Big\{r_n^{(\alpha,\beta)}, w_n^{(\alpha,\beta)}\Big\}$.

In many computations we cannot exactly compute the modal coefficients $\hat{f}_n^{(\alpha,\beta)}$ because we cannot compute the integral exactly, or we can only evaluate f but do not know an analytic form for it. Instead, we can use quadrature rules to approximate the modal coefficients:

$$\hat{f}_n^{(\alpha,\beta)} \simeq \tilde{f}_n^{(\alpha,\beta)} := Q_N^{(\alpha,\beta)}\Big[\, f\,\tilde{P}_n^{(\alpha,\beta)}\Big].$$

We can then form the following approximation to $\mathcal{P}_N^{(\alpha,\beta)} f$:

$$\mathcal{I}_N^{(\alpha,\beta)} := \sum_{n=0}^{N-1} \tilde{f}_n^{(\alpha,\beta)}\,\tilde{P}_n^{(\alpha,\beta)}.$$

Due to the exactness of the Gauss quadrature rule, $\mathcal{I}_N^{(\alpha,\beta)} f = \mathcal{P}_N^{(\alpha,\beta)} f$ for any $f \in \mathcal{B}_N$. Because of the Christoffel-Darboux identity, the expansion $\mathcal{I}_N^{(\alpha,\beta)} f$ is the unique $(N-1)$st degree polynomial interpolant of f at the nodes $\Big\{r_n^{(\alpha,\beta)}\Big\}_{n=1}^{N}$. For $f \notin \mathcal{B}_N$, the difference between the interpolation $\mathcal{I}_N^{(\alpha,\beta)} f$ and the projection $\mathcal{P}_N^{(\alpha,\beta)} f$ is called the aliasing error [16], and arises due to the error in the quadrature rule.

Let $A,\, B \in \mathbb{N}_0$. We define the following discrete approximations to the N modal coefficients $\Big\{\hat{f}_n^{(\alpha+A,\beta+B)}\Big\}_{n=0}^{N-1}$:

$$\tilde{f}_{n;\mathrm{GQ}}^{(\alpha+A,\beta+B)} \;=\; Q_N^{(\alpha+A,\beta+B)}\Big[\, f\,\tilde{P}_n^{(\alpha+A,\beta+B)}\Big] \tag{4.1}$$

$$\tilde{f}_{n;C}^{(\alpha+A,\beta+B)} \;=\; \sum_{m=0}^{A+B} \lambda_{n+m,n}^{(\alpha+A,\beta+B,\alpha,\beta)}\,\tilde{f}_{n+m;\mathrm{GQ}}^{(\alpha,\beta)} \tag{4.2}$$

$$\tilde{f}_{n;\mathrm{DQ}}^{(\alpha+A,\beta+B)} \;=\; Q_N^{(\alpha,\beta)}\Big[\, f\,\tilde{P}_n^{(\alpha+A,\beta+B)}\,\omega^{(A,B)}\Big] \tag{4.3}$$

The modes $\tilde{f}_{n;\mathrm{GQ}}$ are obtained using the Gaussian quadrature native to the expansion class $(\alpha + A,\ \beta + B)$. The modes $\tilde{f}_{n;C}$ are obtained by performing the matrix multiplication in equation (3.6); i.e. the matrix C (or $\hat{C}$) is used to obtain the modes by promoting the lower-class discerte modes from class $(\alpha,\ \beta)$ to class $(\alpha + A,\ \beta + B)$. The last class of modes $\tilde{f}_{n;\mathrm{DQ}}$ are obtained by using a Gaussian quadrature under the weight $\omega^{(\alpha,\beta)}$ to simulate quadrature under the weight $\omega^{(\alpha+A,\beta+B)}$. We call this last expansion one via 'demoted quadrature', which motivates the subscript DQ.

With these three modal definitions, we can define the three expansions $f_i = \sum_{n=0}^{N-1} \tilde{f}_{n;i}^{(\alpha+A,\beta+B)}\ \tilde{P}_n^{(\alpha+A,\beta+B)}$, for i = GQ,C,DQ. Since GQ represents a strict Gaussian quadrature, we know that $f_{\mathrm{GQ}} = \mathcal{I}_N^{(\alpha+A,\beta+B)} f$. By the results of section 3.2 we also know $f_C = f_{\mathrm{GQ}} = \mathcal{I}_N^{(\alpha,\beta)} f$, which we formally state:

Corollary 4.1. *The following relation holds:*

$$f_C^{(\alpha+A,\beta+B)} = \mathcal{I}_N^{(\alpha,\beta)} f.$$

The first two expansions GQ and C are exact for any $f \in \mathcal{B}_N$. The last expansion, DQ, is only exact if $f \in \mathcal{B}_{N-A-B}$. However, it is important to notice that all of the three expansions are different for $f \notin \mathcal{B}_N$ because the aliasing error for each method is different.

4.2 Chebyshev Interpolants

We consider the following problem: Given a function $f(r)$ for $r \in [-1, 1]$, a Jacobi class $(\alpha,\ \beta) = \left(-\frac{1}{2} + A, -\frac{1}{2} + B\right)$, and a maximum modal number N, use an N-point quadrature rule to compute an approximation to the first N modes. A standard practice is to compute the Gauss-Jacobi interpolant $f_{n;\mathrm{GQ}}^{(\alpha,\beta)}$ (4.1) using the Gaussian quadrature native to class $(\alpha,\ \beta)$, or to apply the associated Vandermonde interpolating matrix. The total operation count for either of these equivalent methods is $O\left(N^2\right)$.

However, given the results in section 3, we can instead compute the modes for f in class $\left(-\frac{1}{2}, -\frac{1}{2}\right)$ and then translate them to class $(\alpha,\ \beta)$ using the matrix C (or $\hat{C}$). Computing the modes for f in class $\left(-\frac{1}{2}, -\frac{1}{2}\right)$ (i.e. the Chebyshev modes) can be accomplished with a fast Fourier Transform (FFT) [16]. Therefore, for general classes $\left(-\frac{1}{2} + A, -\frac{1}{2} + B\right)$ with any natural numbers A, B we can compute the modes using an FFT coupled with a sparse matrix-multiply. This results in the function $f_C^{(\alpha,\beta)}$

In the determination of the expansion coefficients $\tilde{f}_{n;\mathrm{GQ}}$ and $\tilde{f}_{n;C}$, we can characterize overhead and online computational times:

Overhead Time (GQ)

- Computation of the quadrature rule. This requires evaluation of the values $\tilde{P}_{n-1}^{(\alpha,\beta)}\left(r_m^{(-1/2,-1/2)}\right)$ for $m, n = 1, ..., N$. The total cost for this is about $O\left(N^2\right)$

Online Time (GQ)

- Performing the quadrature rule evaluation in equation (4.1). This is basically a matrix-vector multiplication requiring $O\left(N^2\right)$ computations.

Overhead Time (C)

- Precomputations for the FFT. This involves a small prime factorization of N and storage of function evaluations.
- Computing the shift to transform standard Fourier modes, the output of the FFT, to the Chebyshev modes that we desire. This is $O(N)$.
- Calculating the entries in the matrix C. This is an $O(N(A+B))$ operation.

Online Time (C)

- Performing the FFT to recover the Fourier modes and transforming them to the Chebyshev modes. $O(N \log N)$
- Multiplication by the sparse matrix C. This requires $O(N(A+B))$ operations.

To summarize, the GQ method has $O\big(N^2\big)$ complexity for both the overhead and online times. The C method is $O(N(\log\ N\ +\ A\ +\ B))$ total. The GQ method produces the modes $\tilde{f}^{(\alpha,\beta)}_{n;\mathrm{GQ}}$, and the C method produces the modes $\tilde{f}^{(\alpha,\beta)}_{n;C}$.

We will use these characterizations of the online and overhead times for our results in the next section.

5 Numerical examples

This section is devoted to presenting quantitative evidence showing that the machinery we have developed is more robust than Gaussian quadrature, and more efficient than direct quadrature methods for computing Jacobi spectral coefficients if 2α and 2β are odd integers.

5.1 Efficiency

In this section we will test the theoretical methods developed in section 3 applied to Chebyshev-Jacobi polynomial expansions $\Big(-\frac{1}{2}+A, -\frac{1}{2}+B\Big)$ as described in section 4.2. We take the test function

$$f(r) = \exp\bigg(-5\Big(r-\frac{\pi}{6}\Big)^2\bigg) + \sin(r),$$

which is analytic but does not exhibit any symmetry on the interval $r \in [-1,1]$. Using the algorithms presented in section 4, we can compute two spectral expansions of f: $f^{(\alpha,\beta)}_{\mathrm{GQ}}$ and $f^{(\alpha,\beta)}_{C}$. We split the computer work required into the 'overhead', and 'online' divisions, which are defined in section 4.2. By performing the algorithms delineated in section 4.2, we can measure the time required to perform spectral expansions using the GQ and C methods.

In figure 5.1 we show the online times for the GQ and C methods for A and B taking values 5 and 10. We see that the online time for the C method with the FFT is relatively insensitive to N, growing only linearly with N. However, the GQ (direct quadrature) method grows with N^2 and is more expensive than the C method. The time spent for the C method is split almost evenly between the FFT and application of the matrix C. Application of C becomes the dominant factor when A and B become large.

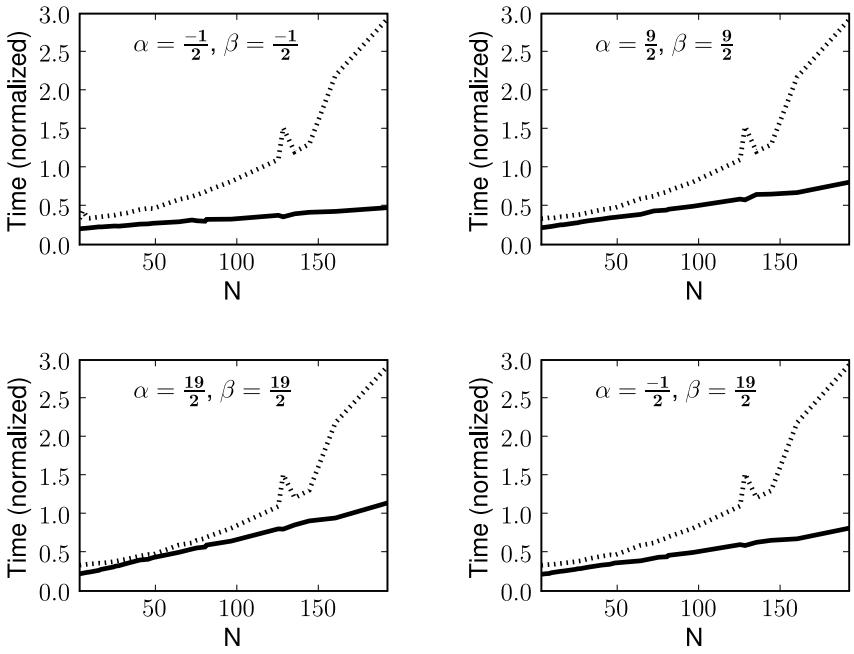

Figure 5.1. Plots of the online times for determining N modal coefficients using N nodal evaluations. FFT+C-matrix calculations are plotted (solid line) vs. direct quadrature calculations (dashed line) for various expansion classes (α, β). The kink around $N = 128$ represents the limitations of the hardware used to perform computations and does not reflect the algorithm complexity.

It is worth noting that the timings in figure 5.1 should be taken with a grain of salt: computational timings for the FFT vs quadrature for small N are extremely sensitive to the method of coding, the particular libraries used, the compiler, and the computer hardware. However, it is clear that for large N the FFT-based approach is undoubtedly faster than a direct application of quadrature, and that this speed advantage remains despite the cost of multiplication by C.

In figure 5.2 we show the same results as in figure 5.1, but we focus on how the parameters A and B affect the online time required for the C method. As expected, the slope of the linear relation between computational time and N is directly related to $A + B$. In the cases $(\alpha, \beta) = \left(\frac{9}{2}, \frac{9}{2}\right)$ and $(\alpha, \beta) = \left(-\frac{1}{2}, \frac{19}{2}\right)$, we have $A + B = 10$, and the online time required is almost identical.

Another topic to consider is the overhead time required to compute the connection matrix for the C method or the quadrature rule for the GQ method. In figure 5.3 we show these results. We see that even for small N the overhead time required for the C method is less than that required for the quadrature method. Note that we have even given the GQ method a bit of an advantage: in section 4.2, we defined the overhead time for the GQ method, and we did *not* include the time required to form the Gaussian quadrature rule nodes and weights $r_n^{(\alpha,\beta)}$ and $w_n^{(\alpha,\beta)}$, respectively. This requires an additional $O(N^2)$ operations (via the Golub-Welsch algorithm); we did not include it because in practice one may not compute f_{GQ}, but instead the demoted quadrature expansion f_{DQ} from equation (4.3) because the Chebyshev-Gauss quadrature rule has an analytic form and is very easy to compute [16]. However, the DQ quadrature becomes more and more inaccurate as A and B are increased if N is fixed. The 'quadrature' overhead time plotted in figure 5.3 is actually that for the DQ method, and not the GQ method.

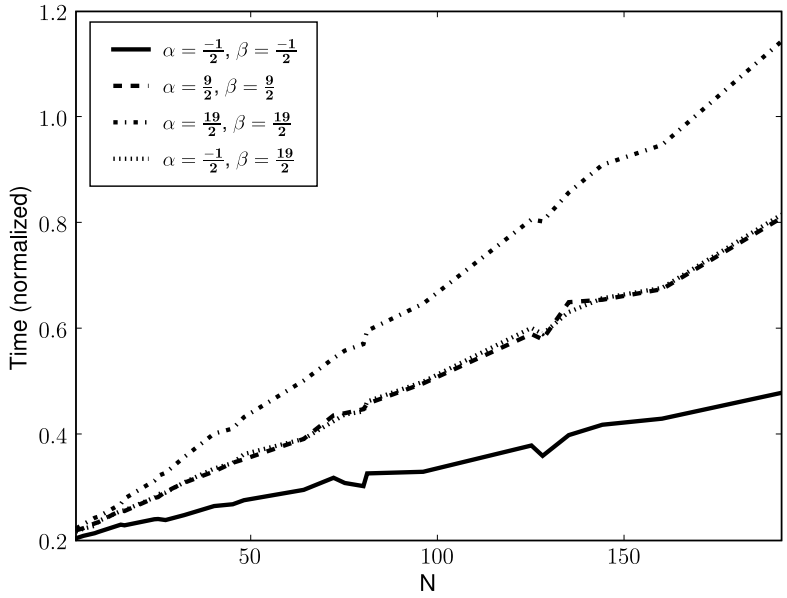

Figure 5.2. Plot of the online computational time required for the C method vs. N. The results plotted are the same as in figure 5.1.

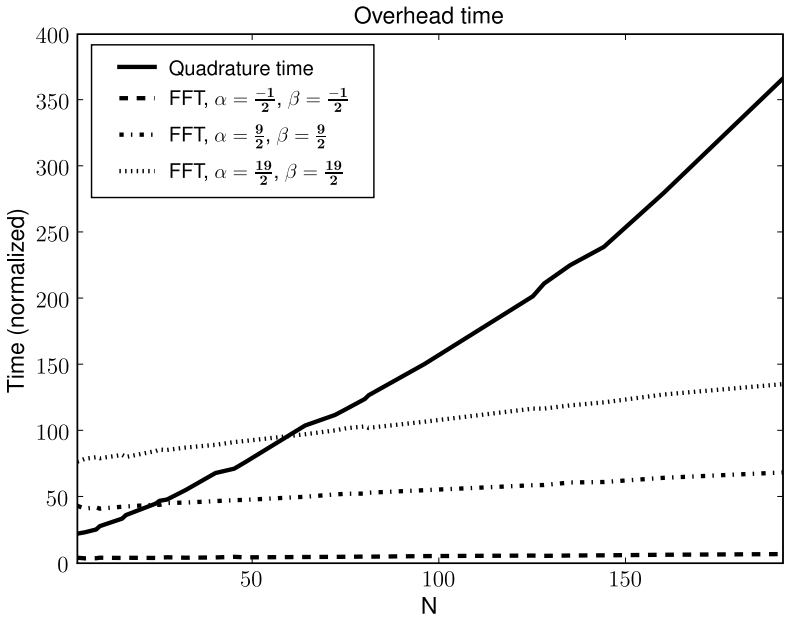

Figure 5.3. Plot of the overhead times vs. number of nodal/modal degrees of freedom N. The overheads are calculated for the f_{GQ} (direct quadrature) and f_C (FFT) methods.

5.2 Accuracy

We present in this section examples to show that an algorithm that judiciously uses the connection coefficients is just as or more accurate than a direct Gaussian quadrature method, and accomplishes the task in much less time. We use the test function

$$f(r) = \sin\Big(q\pi r + \frac{\pi}{4}\Big) = \frac{1}{\sqrt{2}}[\sin(q\pi r) + \cos(q\pi r)], \qquad r \in [-1, 1]. \tag{5.1}$$

If we wish to expand a function $f(r)$ in symmetric Jacobi (i.e. ultraspheric/Gegenbauer) polynomials, we obtain

$$f(r) = \sum_{n=0}^{\infty} \hat{f}_n^{(\alpha,\alpha)} \tilde{P}_n^{(\alpha,\alpha)}(r).$$

In this case, we can find an exact formula for the spectral coefficients. From e.g. Lemma 2.5 in [13] we have:

$$\begin{aligned}\hat{f}_n^{(\alpha,\alpha)} &:= \left\langle f, \tilde{P}_n^{(\alpha,\alpha)} \right\rangle_{(\alpha,\alpha)} \\ &= \frac{1}{\pi^\alpha q^{\alpha+1/2}} \sqrt{\frac{\Gamma(n+2\alpha+1)\,(n+\alpha+1/2)}{n!}} J_{n+\alpha+1/2}(q\pi) \times \begin{cases} (-1)^{(n-1)/2}, & n \text{ odd} \\ (-1)^{n/2}, & n \text{ even,} \end{cases}\end{aligned}$$

where $J_\nu(x)$ is the Bessel function of the first kind. In the case of $\alpha = -\frac{1}{2}$ with $n = 0$, we must divide the above by $\sqrt{2}$. One of the standard ways of numerically obtaining approximations to the modes $\hat{f}_n^{(\alpha,\alpha)}$ is to use the Gaussian quadrature rule $Q_N^{(\alpha,\alpha)}$ native to the Jacobi polynomial class (α, α). The argument we make here is that it is better to determine coefficients to a different Jacobi polynomial class and then use the connection coefficient relations we have derived to obtain the desired modes. Normally we would incur an additional $O\big(N^2\big)$ cost for this procedure, but if we only apply the connection between classes with integral-valued separation, we can accomplish this task in only $O(N)$ cost, which is the result from Theorem 3.2. We thus identify three methods for obtaining approximations to the modes $\left\{\hat{f}_n^{(\alpha,\alpha)}\right\}_{n=0}^{N-1}$, which are derived from the quadrature methods (4.1–4.3):

- Native Gauss quadrature (cf. equation (4.1))
  - Determine the quadrature rule $Q_N^{(\alpha,\alpha)}$
  - Apply $Q_N^{(\alpha,\alpha)}$ to the nodal evaluations $f\Big(r_n^{(\alpha,\alpha)}\Big)$ to obtain approximations to the modes. The function recovered is $\mathcal{I}_N^{(\alpha,\alpha)} f = f_{\mathrm{GQ}}^{(\alpha,\alpha)}$
- Demoted Gauss quadrature (cf. equation (4.3))
  - Define $A := \lceil \alpha \rceil$ and $\underline{\alpha} := \alpha - A \in (-1, 0]$. Determine the quadrature rule $Q_{N+2A}^{(\underline{\alpha},\underline{\alpha})}$
  - Apply $Q_{N+2A}^{(\underline{\alpha},\underline{\alpha})}$ to the nodal evaluations $f\Big(r_n^{(\underline{\alpha},\underline{\alpha})}\Big)\omega^{(A,A)}\Big(r_n^{(\underline{\alpha},\underline{\alpha})}\Big)$ to obtain approximations to the modes N modes $\hat{f}_n^{(\alpha,\alpha)}$. The function recovered is $f_{\mathrm{DQ}}^{(\alpha,\alpha)}$
- Demoted Gauss quadrature + FFT (useful only when $\alpha - \lceil \alpha \rceil = -\frac{1}{2}\Big)$ (cf. equation (4.2))
  - Define $A := \lceil \alpha \rceil$ and $\underline{\alpha} := \alpha - A$. Determine the quadrature rule $Q_{N+2A}^{(\underline{\alpha},\underline{\alpha})}$
  - Apply $Q_{N+2A}^{(\underline{\alpha},\underline{\alpha})}$ to the nodal evaluations $f\Big(r_n^{(\underline{\alpha},\underline{\alpha})}\Big)$ to obtain approximations to the modes $N + 2A$ modes $\hat{f}_n^{(\underline{\alpha},\underline{\alpha})}$. This can be done with the FFT if $\underline{\alpha} = -\frac{1}{2}$. The function recovered here is $\mathcal{I}_{N+2A}^{(\underline{\alpha},\underline{\alpha})} f$.

- Apply the connection matrix $\hat{C}$ to recover $\hat{f}_n^{(\alpha,\alpha)}$, which are the exact modes for the function $\mathcal{P}_N^{(\alpha,\alpha)}\mathcal{I}_{N+2A}^{(\underline{\alpha},\underline{\alpha})}f$.

Note that in the above algorithms we have chosen an N-point quadrature rule for native Gauss quadrature and demoted quadrature, and an $(N+2A)$-point rule for the demoted quadratures; we need the extra nodes for the demoted quadrature rule in order to claim exactness for $f \in \mathcal{B}_N$. While this initially seems like a disadvantage, our results show that the demoted quadrature rule is more accurate than native Gauss quadrature, especially for large α. The reasoning comes from the observation in e.g. [16] that the Gauss quadrature nodal points tend to approach the equidistant nodal set as α is increased. It is well-known that the equidistant nodal set for interpolation produces a much worse quality interpolant than a nodal set where the nodes cluster near the boundaries.

Take specifically the case when $\alpha = -\frac{1}{2} + A$ and $\beta = -\frac{1}{2} + B$. We know that $f_{\mathrm{GQ}} = \mathcal{I}_N^{(\alpha,\beta)}f$, and from Corollary 4.1 that $f_C = \mathcal{I}_N^{(-1/2,-1/2)}f$. Again, the nodes $\left\{r_n^{(\alpha,\beta)}\right\}_{n=1}^N$ approach the equidistant nodal set as α and β are increased. The equidistant nodal set for polynomial interpolation has an exponentially growing Lebesgue constant [18], whose magnitude bounds the maximum pointwise error of an interpolant. Because large $(\alpha,\ \beta)$ will yield an interpolant f_{GQ} on near-equidistant nodes, we have good reason to suspect that f_{GQ} will be a bad pointwise estimator for the function f. By contrast, it is also known that the Chebyshev-Gauss nodes have a nearly-optimal Lebesgue constant [15], of order $\log(N)$. Therefore, the function f_C is an orders-of-magnitude better pointwise interpolant than f_{GQ} for large $\alpha,\ \beta$, especially near the endpoints of the interval (i.e. the Runge phenomenon). This is why we 'demote' α to $\underline{\alpha}$ in order to obtain a better nodal set for interpolation (even when $\underline{\alpha} \neq -1/2$).

We recall that the last $A+B$ modes of the f_C expansion are incomplete in information. Therefore, if one discards these last few modes (effectively using $\hat{C}$ instead of C) then we have an approximation to $\mathcal{P}_N^{(-1/2+A,-1/2+B)}f$. However, it is also known that for large A, B that projection also exhibits very ill-behaved oscillations; this is termed the generalized Runge phenomenon [7]. This is not something we discuss further in this paper.

Returing to the case when $\underline{\alpha} = -\frac{1}{2}$, we can use the FFT for the demoted quadrature rule (since then $Q_N^{(\underline{\alpha},\underline{\alpha})}$ is the Chebyshev quadrature rule), which mitigates the marginal increase in computational cost of using $N+2A$ modes. Thus, we have strong reason to believe that using the demoted quadrature rule has accuracy advantages over the native Gauss rule, and if $\underline{\alpha} = -\frac{1}{2}$, the small increase in cost is largely offset by the usage of the FFT.

To quantitatively validate these claims, we assume that we obtain a function g using one of the above methods, and we introduce an error measure $\varepsilon_{\mathrm{rel}}$ defined as

$$\varepsilon_{\mathrm{rel}} = \frac{\left\| \mathcal{P}_N^{(\alpha,\alpha)}f - g \right\|_{(\alpha,\alpha)}}{\left\| \mathcal{P}_N^{(\alpha,\alpha)}f \right\|_{(\alpha,\alpha)}}.$$

In figure 5.4 we show the scaled error $\varepsilon_{\mathrm{rel}}$ as a function of α for the function f in (5.1) with $q = 80$ for the native Gauss quadrature and demoted quadrature methods. We have used 500 quadrature points (for both methods) and $N = 300$ modes were computed. For large values of α, the the Gauss rule produces ill-conditioned results, whereas the demoted quadrature rule can provide very accurate modal information for $\underline{\alpha}$ that can be promoted robustly to modal information for α using $\hat{C}$.

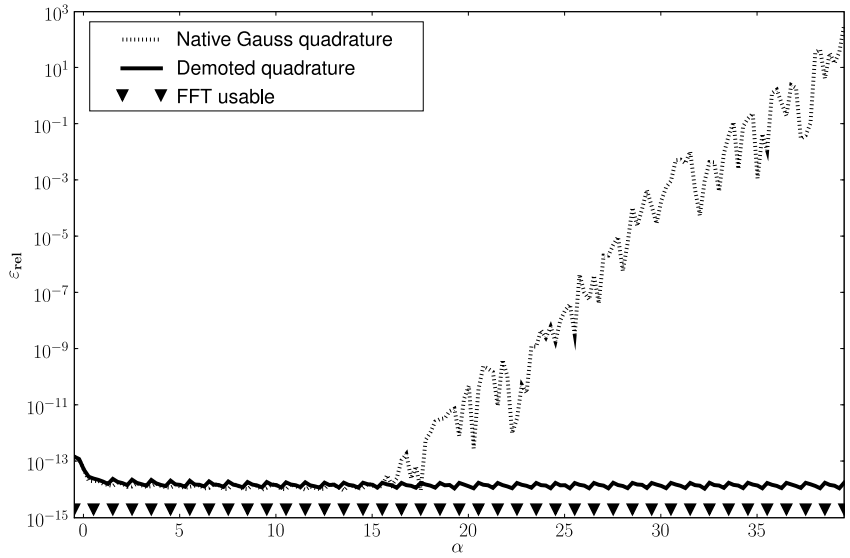

Figure 5.4. The relative error ε_{rel} for the native Gauss and demoted quadrature rule methods. 500 interpolation points are used in both cases, and $N = 300$ modes are computed.

In addition, we tabulate ε_{rel} and computational times in table 5.1 for various values of α for which $\underline{\alpha} = -\frac{1}{2}$. Using demoted quadrature in conjunction with the FFT is both more accurate and much faster than using native Gauss quadrature. Although the error for the native Gauss rule does not seem significant for $\alpha \lesssim 20$, a modification of the parameter q in equation (5.1) can greatly exacerbate the accuracy problem for Gauss quadrature and further motivates the desire to use the demoted quadrature rule, even for small α.

ε_{rel} error

	Native Gauss	Demoted	Demoted + FFT*
$\alpha = -0.5$	1.495 E-13	1.495 E-13	3.228 E-14
$\alpha = 9.5$	1.170 E-14	1.869 E-14	4.422 E-14
$\alpha = 19.5$	8.142 E-13	1.739 E-14	4.475 E-14
$\alpha = 29.5$	1.197 E-04	1.729 E-14	4.509 E-14
$\alpha = 39.5$	3.347 E+02	1.759 E-14	4.556 E-14

Computational Time (s)

	Native Gauss	Demoted	Demoted + FFT*
$\alpha = -0.5$	0.326	0.323	0.001
$\alpha = 9.5$	1.156	0.324	0.009
$\alpha = 19.5$	1.187	0.327	0.018
$\alpha = 29.5$	1.209	0.325	0.025
$\alpha = 39.5$	1.225	0.327	0.032

Table 5.1. ε_{rel} and computational time tabulations for various values of α. ($*$ FFT only available when $\underline{\alpha} = -\frac{1}{2}$).

Finally, we note that the FFT can be more accurate than direct methods if accurate methods are employed to compute the overhead sine/cosine table factors [21]. We have not made an attempt to verify the accuracy of our FFT code against direct methods. However, the argument that the FFT is more accurate than direct methods (if implemented propertly), along with the observation that demoted quadrature yields more accurate results than native Gauss quadrature, makes a strong case for both the stability and efficiency of our proposed method.

6 Summary

We have presented an inexpensive algorithm for transforming modal coefficients of a Jacobi polynomial expansion of class (α, β) to the modal coefficients of class $(\alpha + A, \beta + B)$ for $A, B \in \mathbb{N}_0$. Such an exact transformation is possible due to the sparsity of the connection coefficients relating different Jacobi polynomial classes. This transformation can also be efficiently implemented, transforming N modes in $O(N(A + B))$ computations. In the case where $\alpha = \beta = -\frac{1}{2}$, one can apply the FFT to compute modal expansions of class $\left(-\frac{1}{2} + A, -\frac{1}{2} + B\right)$ in $O(N \log N)$ time. For large N and large A and B the FFT algorithm proves to be a more efficient method for computing modal coefficients than direct quadrature. In addition, we observe that using 'demoted quadrature' produces much more accurate results than using 'native Gauss quadrature', which we attribute to the decreased pointwise accuracy of the Gauss interpolant versus the demoted quadrature interpolant.

Although our numerical examples have concentrated on the Jacobi-Gauss quadrature, the method is equally applicable to the Radau and Lobatto quadratures as well, since Chebyshev-Gauss-Radau and Chebyshev-Gauss-Lobatto quadrature rules are FFT-implementable as well. In addition, fast algorithms for Legendre polynomial expansions also exist (e.g. [2], [9], [10]), which means that this algorithm also yields asymptotically $O(N \log N)$ spectral transformations for polynomial expansions in any class of the form (A, B) as well when combined with one of the fast Legendre algorithms. We also note that Boyd provides the possibility of using the fast multipole method (FMM) for evaluating modal coefficients on Gaussian quadrature nodes [6]. This enables the possibility of an $O(N \log N)$ algorithm for the Gauss quadrature method as well; but as mentioned in [6], while the FMM has the same asymptotic complexity as the FFT, it unfortunately has a much larger constant of proportionality than the FFT, so the FFT is vastly superior if one can use it.

There is still room for improvement for our method: we have used packaged FFT routines, but for our purpose of calculating Chebyshev modes, the method is more efficient if instead we use fast cosine transform routines. In addition, we have assumed for given A and B that exactly $(A + B + 1)\left(N - \frac{(A+B)}{2}\right)$ elements of C are nonzero (that is, the first $A + B + 1$ superdiagonals). However, if $\alpha = \beta$ and $A = B$, then the odd superdiagonals are actually zero (this symmetry in the connection coefficients for Gegenbauer polynomials is known [4]) . This means that an online application of C for Gegenbauer/Ultraspheric expansions can be optimized by a factor of roughly 2, which we have not done in this paper. Because application of C is usually on the same order of magnitude as application of the FFT, this is can result in a significant speedup of the method.

Finally, the inverse transform from modes of order $\left(-\frac{1}{2} + A, -\frac{1}{2} + B\right)$ to Chebyshev-Gauss(-Radau/Lobatto) nodes is also possible via the FFT: one must back-substitute to solve the system

$$\tilde{\boldsymbol{f}}^{(\boldsymbol{\alpha}+\boldsymbol{A},\boldsymbol{\beta}+\boldsymbol{B})} = C\tilde{\boldsymbol{f}}^{(\boldsymbol{\alpha},\boldsymbol{\beta})},$$

for the modes $\tilde{f}^{(\alpha,\beta)}$, which is a sequential operation with nearly the same number of operations as the forward application of C. (Recall by proposition 3.4 that C is invertible.) Then if $\alpha = \beta = -\frac{1}{2}$, one can use the FFT to recover the nodal evaluations.

Python code used to generate the figures is available upon request.

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Appendix A Jacobi polynomial properties

This appendix is devoted to providing the formulae necessary to carry out the algorithms presented in this paper. The Jacobi polynomials satisfy recurrence relations (2.5)-(2.8) for the constants $\mu_{n,0/1}^{(\alpha,\beta)}$ and $\nu_{n,0/1}^{(\alpha,\beta)}$. To derive these constants, we note that the usual scaling found for the Jacobi polynomials is that adhering to the criterion

$$\hat{P}_n^{(\alpha,\beta)}(r=1) = \begin{pmatrix} n+\alpha \\ n \end{pmatrix},$$

where we have introduced the scaled Jacobi polynomials $\hat{P}_n^{(\alpha,\beta)}$, which are the scaled polynomials that usually appear in the literature [1]. From various sources, e.g. [22], we have that these polynomials satisfy promotion and demotion formulae in a form similar to (2.5)-(2.8), but with different constants. With these formulae from the literature, we have that the *monic* Jacobi polynomials $P_n^{(\alpha,\beta)}$ satisfy the same promotion and demotion formulae with the constants:

$$\begin{aligned}
(1-r)P_n^{(\alpha,\beta)} &= \frac{2(n+\alpha)(n+\alpha+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)} P_n^{(\alpha-1,\beta)} - P_{n+1}^{(\alpha-1,\beta)} \\
(1+r)P_n^{(\alpha,\beta)} &= \frac{2(n+\beta)(n+\alpha+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)} P_n^{(\alpha,\beta-1)} + P_{n+1}^{(\alpha,\beta-1)} \\
P_n^{(\alpha,\beta)} &= P_n^{(\alpha+1,\beta)} - \frac{2n(n+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)} P_{n-1}^{(\alpha+1,\beta)} \\
P_n^{(\alpha,\beta)} &= P_n^{(\alpha,\beta+1)} + \frac{2n(n+\alpha)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)} P_{n-1}^{(\alpha,\beta+1)}
\end{aligned}$$

The monic polynomials have norm $\left\| P_n^{(\alpha,\beta)} \right\|^2 = h_n^{(\alpha,\beta)}$, which is given by

$$h_n^{(\alpha,\beta)} = \frac{2^{2n+\alpha+\beta+1}(n!)\,\Gamma(n+\alpha+\beta+1)\,\Gamma(n+\alpha+1)\,\Gamma(n+\beta+1)}{\Gamma(2n+\alpha+\beta+1)\,\Gamma(2n+\alpha+\beta+2)}, \tag{A.1}$$

where $\Gamma(\,\cdot\,)$ represents the Gamma function. The above formulae allow us to translate the promotion/demotion formulae for the monic polynomials into those for the normalized Jacobi polynomials, as given in equations (2.5)-(2.8). After some algebra, we determine that the constants in those equations are given by

$$\mu_{n,0}^{(\alpha,\beta)} = \sqrt{\frac{2(n+\alpha)(n+\alpha+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)}} \tag{A.2}$$

$$\mu_{n,1}^{(\alpha,\beta)} = \sqrt{\frac{2(n+1)(n+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)}} \tag{A.3}$$

$$\nu_{n,0}^{(\alpha,\beta)} = \sqrt{\frac{2(n+\alpha+1)(n+\alpha+\beta+1)}{(2n+\alpha+\beta+1)(2n+\alpha+\beta+2)}} \tag{A.4}$$

$$\nu_{n,-1}^{(\alpha,\beta)} = \sqrt{\frac{2n(n+\beta)}{(2n+\alpha+\beta)(2n+\alpha+\beta+1)}} \tag{A.5}$$

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