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Chebyshev Polynomials in the Spectral Tau Method and Applications to Eigenvalue Problems

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1. Introduction

Chebyshev Spectral Tau methods are a useful technique for solving ordinary differential equations. Numerical programs using this method are often considerably faster with greater accuracy than other standard techniques such as finite differencing. In my attempt to understand Chebyshev polynomials and their applications, I was unable to find one definitive book or article which took me from only a general knowledge of calculus and linear algebra to being able to confidently apply these new techniques. This tutorial is an attempt to fill that need. Several examples are worked out to demonstrate the usefulness and occasional difficulty of their application.

This series has been broken down into four major parts. Section one gives a brief explanation and example of when and why Chebyshev Polynomials are so useful. The second section is a detailed account of the definitions, properties and algebra that surrounds Chebyshev Polynomials. Because section two is so detailed, the reader may read only the first few and last few paragraphs to get an overview of its material. Section three is also a detailed piece. It deals with the recurrence relationship between functions and Chebyshev Polynomials. These recurrence relationships are very important in the implementation of Chebyshev Polynomials to spectral methods. None the less, most of the common recurrence relationships are tabulated in the appendix of Gottlieb and Orszag's book [4]. For this reason, the hurried reader may just browse over the third section. Section four gives several examples of how to implement Chebyshev Polynomials with spectral tau methods. All the examples are linear differential equations and most involve finding the eigenvalues of these equations.

It can be shown that the coefficient on the x^n term of the Chebyshev polynomial is 2^{n-1} . This is left as an exercise in Exercise 2.3. In this tutorial we will take some function, truncate it and expand it in terms of a Chebyshev Polynomial. When a function is expanded in terms of some other polynomial, the coefficients of the expansion are roughly inversely proportional to the coefficients of the polynomial. Therefore, a function expanded in terms of a Chebyshev Polynomial will have coefficients roughly proportional to 2^{1-n} . This gives a geometric rate of convergence as the number of terms in the expansion, n , is increased. The following example¹ is taken from an excellent source for spectral methods, *Spectral Methods in Fluid Dynamics* [2]. The example deals with a linear heat equation with

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homogeneous Dirichlet boundary conditions, over the interval of $[-1, 1]$.

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0 \quad (1.1)$$

$$u(1, t) = 0 \quad (1.2)$$

$$u(-1, t) = 0 \quad (1.3)$$

$$u(x, 0) = \sin \pi x \quad (1.4)$$

A Chebyshev collocation method and a second order difference equation are used to solve for u . The convergence of the two compared to the number of terms is given in the table below.

Table 1.1 Maximum error for the one-dimensional heat equation

N	Chebyshev collocation	Second Order finite difference
8	$4.58 * 10^{-4}$	$6.44 * 10^{-1}$
10	$8.25 * 10^{-6}$	$3.59 * 10^{-1}$
12	$1.01 * 10^{-7}$	$2.50 * 10^{-1}$
14	$1.10 * 10^{-9}$	$1.74 * 10^{-1}$
16	$2.09 * 10^{-11}$	$1.35 * 10^{-1}$

Looking at the errors between the two methods, it becomes rather obvious that the Chebyshev method converges significantly faster. This faster convergence rate would produce enormous savings in computational time.

2. Chebyshev Polynomials

2.1. Definition

The Chebyshev polynomial is defined as

$$T_n(x) = \cos [n \arccos(x)] \quad (2.1)$$

$$-1 \leq x \leq 1 \quad (2.2)$$

$$x = \cos \theta \quad (2.3)$$

2.2. Minima and Zeroes

The minima are the values in which the Chebyshev polynomial is equal to zero.

$$T_n(x) = 0 = \cos(n\theta) \quad (2.4)$$

$$\cos(n\theta_j) = 0 \quad \theta_j = \frac{2j-1}{n} \frac{\pi}{2} \quad \text{for } j = 1, 2, \dots, n$$

2.3. Extrema

$|T_n(x)| = 1$ is the extrema of $T_n(x)$

$$|T_n(\eta_k)| = 1 \quad \eta_k = \cos\left(\frac{k\pi}{n}\right) \quad \text{for } k = 1, 2, \dots, n \quad (2.5)$$

$$T_n(\pm 1) = (\pm 1)^n \quad (2.6)$$

2.4. Polynomial Expression

A simple method for finding Chebyshev polynomial expressions can be done using trigonometry and a recurrence relation. Start with the first two polynomials, $T_0(x) = \cos 0 = 1$, and $T_1(x) = \cos \theta = x$. From the relation

$$2 \cos \theta \cos n\theta = \cos(n+1)\theta + \cos(n-1)\theta \quad (2.7)$$

$$2xT_n(x) = T_{n+1}(x) + T_{n-1}(x)$$

$$T_{n+1}(x) = 2xT_n(x) - T_{n-1}(x) \quad (2.8)$$

$$T_2(x) = 2xT_1(x) - T_0(x) = 2x^2 - 1$$

$$T_3(x) = 2xT_2(x) - T_1(x) = 4x^3 - 3x$$

This method of arriving at the n^{th} degree polynomial is preferred when writing computer programs[12].

The following is a more rigorous method for determining Chebyshev Polynomials of any degree. First write out DeMoivre's Theorem.

$$e^{i\theta} = \cos \theta + i \sin \theta$$

$$e^{in\theta} = (\cos \theta + i \sin \theta)^n = \cos(n\theta) + i \sin(n\theta) \quad (2.9)$$

by the binomial expansion,

$$\begin{aligned} (\cos \theta + i \sin \theta)^n &= \cos^n \theta + \binom{n}{1} \cos^{n-1} \theta (i \sin \theta) + \\ &\quad \binom{n}{2} \cos^{n-2} \theta (i \sin \theta)^2 + \dots + \binom{n}{n} (i \sin \theta)^n \end{aligned} \quad (2.10)$$

Equating the real parts of (2.10) gives

$$\begin{aligned} \cos n\theta &= \cos^n \theta + \binom{n}{2} \cos^{n-2} \theta (i \sin \theta)^2 + \binom{n}{4} \cos^{n-4} \theta (i \sin \theta)^4 \\ &\quad + \dots + \binom{n}{\eta} \cos^{n-2\eta} \theta (i \sin \theta)^{2\eta} \end{aligned} \quad (2.11)$$

where

$$\eta = \left[\frac{n}{2} \right] = \begin{cases} \frac{n}{2} & n \text{ is even} \\ \frac{n-1}{2} & n \text{ is odd} \end{cases} \quad (2.12)$$

substituting $\sin^2 \theta = 1 - \cos^2 \theta$

$$\begin{aligned} \cos n\theta &= \cos^n \theta - \binom{n}{2} \cos^{n-2} \theta (1 - \cos^2 \theta) + \binom{n}{4} \cos^{n-4} \theta (1 - \cos^2 \theta)^2 \\ &\quad + \cdots + (-1)^\eta \binom{n}{\eta} \cos^{n-2\eta} \theta (1 - \cos^2 \theta)^\eta \end{aligned} \quad (2.13)$$

$$\begin{aligned} \cos n\theta &= \cos^n \theta - \binom{n}{2} \cos^{n-2} \theta + \binom{n}{2} \cos^n \theta \\ &\quad + \binom{n}{4} \cos^{n-4} \theta - 2 \binom{n}{4} \cos^{n-2} \theta + \binom{n}{4} \cos^n \theta + \cdots \\ \cos n\theta &= \sum_{j=0}^{\eta} (-1)^j \binom{n}{2j} \cos^{n-2j} \theta \left[\sum_{k=0}^j (-1)^k \binom{j}{k} \cos^{2k} \theta \right] \end{aligned} \quad (2.14)$$

The summation can be reordered by letting

$$A_j = (-1)^j \binom{n}{2j} \cos^{n-2j} \theta \quad B_{kj} = (-1)^k \binom{j}{k} \cos^{2k} \theta$$

$$\begin{aligned} \cos n\theta &= \sum_{j=0}^{\eta} A_j \sum_{k=0}^j B_{kj} = \sum_{j=0}^{\eta} A_j [B_{0j} + B_{1j} + \cdots + B_{jj}] \\ &= A_0 [B_{00}] \\ &\quad + A_1 [B_{01} + B_{11}] \\ &\quad + A_2 [B_{02} + B_{12} + B_{22}] \\ &\quad \vdots \\ &\quad + A_q [B_{0q} + B_{1q} + \cdots + B_{qq}] \\ &\quad \vdots \\ &\quad + A_\eta [B_{0\eta} + B_{2\eta} + \cdots + B_{\eta\eta}] \end{aligned} \quad (2.15)$$

Factor the B_{kj} terms

$$\begin{aligned}
& B_{00} [A_0] + B_{01}A_1 + B_{02}A_2 + \cdots + B_{0\eta}A_\eta \\
& + B_{11}A_1 + B_{12}A_2 + \cdots + B_{1\eta}A_\eta \\
& \quad \vdots \\
& + B_{qq}A_q + B_{q,q+1}A_{q+1} + B_{q,q+2}A_{q+2} + \cdots + B_{q\eta}A_\eta \\
& \quad \vdots \\
& + B_{\eta-1,\eta-1}A_{\eta-1} + B_{\eta-1,\eta}A_\eta \\
& + B_{\eta\eta}A_\eta \tag{2.16} \\
= & \sum_{k=j}^{\eta} B_{jk}A_k \quad \text{for } j = 0, 1, 2, \dots, \eta
\end{aligned}$$

$$= \sum_{j=0}^{\eta} \sum_{k=j}^{\eta} B_{jk}A_k \tag{2.17}$$

Substituting back in the expressions for A_k and B_{jk} gives

$$\begin{aligned}
& \sum_{j=0}^{\eta} \sum_{k=j}^{\eta} \left[(-1)^j \binom{k}{j} \cos^{2j} \theta \right] \left[(-1)^k \binom{n}{2k} \cos^{n-2k} \theta \right] \\
= & \sum_{j=0}^{\eta} (-1)^j \cos^{2j} \theta \sum_{k=j}^{\eta} \left[(-1)^k \binom{n}{2k} \binom{k}{j} \cos^{n-2k} \theta \right] \\
= & \sum_{j=0}^{\eta} (-1)^j \cos^{2j} \theta \left[(-1)^j \binom{n}{2j} \binom{j}{j} \cos^{n-2j} \theta \right. \\
& + (-1)^{j+1} \binom{n}{2(j+1)} \binom{j+1}{j} \cos^{n-2(j+1)} \theta + \dots \\
& + (-1)^{j+q} \binom{n}{2(j+q)} \binom{j+q}{j} \cos^{n-2(j+q)} \theta + \dots \\
& \left. + (-1)^{\eta} \binom{n}{2\eta} \binom{\eta}{j} \cos^{n-2\eta} \theta \right] \\
= & \sum_{j=0}^{\eta} (-1)^{2j+q} \binom{n}{2(j+q)} \binom{j+q}{j} \cos^{n-2q} \theta \quad \text{for } q = 0, 1, \dots, n \tag{2.18}
\end{aligned}$$

showing that $(-1)^{2j+q} = (-1)^{2j}(-1)^q = (-1)^q$ gives the final expression for the Chebyshev polynomial of degree n .

$$T_n(x) = \cos n\theta = \sum_{k=0}^n (-1)^k \sum_{j=k}^n \binom{n}{2j} \binom{j}{k} \cos^{n-2k} \theta \quad (2.19)$$

substituting for $x = \cos \theta$

$$\begin{aligned} T_n(x) &= t_0 + t_1 x + \cdots + t_n x^n \\ t_{n-(2k+1)} &= 0 && \text{for } k = 0, \dots, \left\lfloor \frac{n-1}{2} \right\rfloor \\ t_{n-2k} &= (-1)^k \sum_{j=k}^{\lfloor \frac{n}{2} \rfloor} \binom{n}{2j} \binom{j}{k} && \text{for } k = 0, \dots, \left\lfloor \frac{n}{2} \right\rfloor \end{aligned} \quad (2.20)$$

The above equation states that if n is even then all powers of x are also even and if n is odd then all powers of x are odd. The first few polynomials are given below.

$$\begin{aligned} T_0(x) &= 1 & T_2(x) &= 2x^2 - 1 & T_4(x) &= 8x^4 - 8x^2 + 1 \\ T_1(x) &= x & T_3(x) &= 4x^3 - 3x & T_5(x) &= 16x^5 - 20x^3 + 5x \end{aligned}$$

2.5. Methods of Summation

In the next section, certain recurrence relationships involving derivatives of Chebyshev polynomials will arise. These recurrence formulas will give a rather complicated summation expression. To properly deal with these summations, a technique known as **methods of the summation** [11] will now be introduced.

To begin, we first define the difference operator

$$\Delta f(x) = f(x+h) - f(x) \quad (2.21)$$

and let $h = 1$.

$$\Delta f(x) = f(x+1) - f(x) \quad (2.22)$$

The difference operator Δ is a linear operator and behaves similarly (but not exactly) to a differential operator.

$$\Delta [af(x) + bg(x)] = a\Delta f(x) + b\Delta g(x) \quad (2.23)$$

$$\begin{aligned}\Delta [f(x)g(x)] &= f(x+1)g(x+1) - f(x)g(x) \\ &\quad - [f(x+1)g(x) - f(x+1)g(x)]\end{aligned}\tag{2.24}$$

$$\begin{aligned}&= f(x+1)[g(x+1) - g(x)] + g(x)[f(x+1) - f(x)] \\ \Delta [f(x)g(x)] &= f(x+1)\Delta g(x) + g(x)\Delta f(x)\end{aligned}\tag{2.25}$$

Similarly

$$\Delta \frac{f(x)}{g(x)} = \frac{g(x)\Delta f(x) - f(x)\Delta g(x)}{g(x+1)g(x)}\tag{2.26}$$

Here are some examples.

$$\begin{aligned}\Delta c &= 0 \\ \Delta x &= 1 \\ \Delta x^2 &= 2x + 1 \\ \Delta x^3 &= 3x^2 + 3x + 1\end{aligned}$$

where $c = \text{constant}$ and n is a positive integer.

Repeated operations give

$$\begin{aligned}\Delta^2 x^2 &= \Delta(\Delta x^2) = \Delta(2x + 1) = 2 \\ \Delta^3 x^2 &= \Delta(2) = 0\end{aligned}$$

in general $\Delta^n cx^n = cn!$ and $\Delta^m cx^m = 0$ for $m > n$.

Now we shall introduce the anti-difference operator Δ^{-1}

$$\text{if } \Delta g(x) = f(x)$$

then

$$\begin{aligned}g(x) &= \Delta^{-1}f(x) \\ \Delta\Delta^{-1}f(x) &= \Delta g(x) \\ f(x) &= \Delta g(x)\end{aligned}$$

Note that $\Delta\Delta^{-1} = 1$ but $\Delta^{-1}\Delta \neq 1!$ That is to say the operations do not commute.

$$\Delta [\Delta^{-1}f(x)] = f(x) \quad \Delta^{-1}[\Delta f(x)] = f(x) + c\tag{2.27}$$

where c is some constant.

Example 2.1. Verify that $\Delta^{-1}x = \frac{1}{2}(x^2 - x) + c$

$$\begin{aligned}\Delta\Delta^{-1}x &= \Delta\left[\frac{1}{2}(x^2 - x) + c\right] \\ &= \frac{1}{2}\Delta x^2 - \frac{1}{2}\Delta x \\ &= x + \frac{1}{2} - \frac{1}{2} = x\end{aligned}$$

Now we will introduce some notation on factorial products.

$$x^{(n)} \equiv x(x-1)(x-2)\cdots(x-n+2)(x-n+1) \quad (2.28)$$

$x^{(n)}$ is called the n^{th} factorial of x . Below is a list of the first few factorials.

$$\begin{aligned}x^{(1)} &= x \\ x^{(2)} &= x(x-1) = x^2 - x \\ x^{(3)} &= x(x-2)(x-1) = x^3 - 3x^2 + 2x\end{aligned}$$

the difference operator of these factorials are

$$\begin{aligned}\Delta x^{(1)} &= \Delta x = 1 \\ \Delta x^{(2)} &= \Delta(x^2 - x) = 2x = 2x^{(1)} \\ \Delta x^{(3)} &= \Delta(x^3 - 3x^2 + 2x) = 3(x^2 - x) = 3x^{(2)}\end{aligned}$$

in general $\Delta x^{(n)} = nx^{(n-1)}$

The n^{th} factorial of x , $x^{(n)}$, can be given in terms of a polynomial expression.

$$x^{(n)} = S_n^{(n)}x^n + S_n^{(n-1)}x^{n-1} + S_n^{(n-2)}x^{n-2} + \cdots + S_n^{(1)}x + S_n^{(0)} = \sum_{m=0}^n S_n^{(m)}x^{(m)} \quad (2.29)$$

the set $\{S_n^{(0)}, S_n^{(1)}, \dots, S_n^{(n)}\}$ is known as Sterling's Numbers of the first kind. Likewise, any power of x can be represented by a polynomial of factorials.

$$x^n = \mathfrak{S}_n^{(n)}x^{(n)} + \mathfrak{S}_n^{(n-1)}x^{(n-1)} + \cdots + \mathfrak{S}_n^{(1)}x^{(1)} + \mathfrak{S}_n^{(0)} = \sum_{m=0}^n \mathfrak{S}_n^{(m)}x^{(m)} \quad (2.30)$$

The set $\{\mathfrak{S}_n^{(0)}, \mathfrak{S}_n^{(1)}, \dots, \mathfrak{S}_n^{(n)}\}$ is known as Sterling's Numbers of the second kind. An excellent source for listing a large number of Sterling's Numbers is given in

the *Handbook of Mathematical Functions*[6]. A list of the first few of Sterling's Numbers of the first and second kind are given below.

$$\begin{array}{ll}
 x^{(0)} = 1 & x^0 = 1 = x^{(0)} \\
 x^{(1)} = x & x^1 = x^{(1)} \\
 x^{(2)} = x^2 - x & x^2 = x^{(2)} + x^{(1)} \\
 x^{(3)} = x^3 - 3x^2 + 2x & x^3 = x^{(3)} + 3x^{(2)} + x^{(1)} \\
 x^{(4)} = x^4 - 6x^3 + 11x^2 - 6x & x^4 = x^{(4)} + 6x^{(3)} + 7x^{(2)} + x \\
 x^{(5)} = x^5 - 10x^4 + 35x^3 - 50x^2 + 24x & x^5 = x^{(5)} + 10x^{(4)} + 25x^{(3)} + 15x^{(2)} + x
 \end{array}$$

The introduction of the difference operator and the factorial notation will now be used together to show a convenient way of solving for the limits of summations. Look at a simple combination of the difference operator and a summation sign.

$$\begin{aligned}
 \sum_{x=1}^4 \Delta f(x) &= \sum_{x=1}^4 [f(x+1) - f(x)] \\
 &= [f(5) + f(4) + f(3) + f(2)] - [f(4) + f(3) + f(2) + f(1)] \\
 &= f(5) - f(1) = f(x) \Big|_{x=1}^{x=5}
 \end{aligned}$$

in general

$$\sum_{x=a}^b \Delta f(x) = f(x) \Big|_{x=a}^{x=b+1} \tag{2.31}$$

Now let $\Delta f(x) = g(x)$

$$\begin{aligned}
 f(x) &= \Delta^{-1}g(x) + c \\
 \sum_{x=a}^b \Delta f(x) &= \sum_{x=a}^b g(x) = f(x) \Big|_{x=a}^{x=b+1} = \Delta^{-1}g(x) + c \Big|_{x=a}^{x=b+1} = \Delta^{-1}g(x) \Big|_{x=a}^{x=b+1}
 \end{aligned}$$

Therefore

$$\sum_{x=a}^b g(x) = \Delta^{-1}g(x) \Big|_{x=a}^{x=b+1} \tag{2.32}$$

This formula gives a method of taking a function under summation and finding its limit assuming one exists and its anti-difference operator can be found.

Example 2.2.

$$\sum_{x=1}^n x^2 = \sum_{x=1}^n (x^{(2)} + x^{(1)})$$

$$x^{(m)} = \Delta \frac{x^{(m+1)}}{m+1} \text{ so } x^{(2)} = \Delta \frac{x^3}{3} \text{ and } x^{(1)} = \Delta \frac{x^2}{2}$$

$$\begin{aligned} \sum_{x=1}^n \Delta \left(\frac{x^{(3)}}{3} + \frac{x^{(2)}}{2} \right) &= \left[\frac{x^{(3)}}{3} + \frac{x^{(2)}}{2} \right] \Big|_{x=1}^{x=n+1} \\ &= \frac{(n+1)^{(3)}}{3} + \frac{(n+1)^{(2)}}{2} - \frac{1^{(3)}}{3} - \frac{1^{(2)}}{2} \\ &= \frac{(n+1)^{(3)}}{3} + \frac{(n+1)^{(2)}}{2} \\ &= \frac{(n+1)(n)(n-1)}{3} + \frac{(n+1)(n)}{2} \\ \sum_{x=1}^n x^2 &= \frac{(2n+1)(n+1)n}{6} \end{aligned}$$

Section 2.1 through 2.4 introduced the definition and some of the properties of Chebyshev Polynomials as well as a derivation of the polynomial itself. Section 2.5 showed a nice trick for evaluating summations which have limits and an antidifference operator. The definition and properties of Chebyshev Polynomials were given to aid anyone interested in more detailed derivations. Section 2.5 will be used in section 3, particularly section 3.2, where recurrence relationships between functions expanded in terms of Chebyshev Polynomials and linear differential operators of these functions, will be dealt with.

2.6. Problems

Exercise 2.1. Find the first four powers of x in terms of $T_n(x)$ by a recurrence relation.

Exercise 2.2. Prove that $T_n(x)$ is commutable; that is $T_r(T_s(x)) = T_{rs}(x) = T_{sr}(x)$. Note that there exists one and only one polynomial which is commutable with $T_n(x)$. Therefore if a polynomial $p_n(x)$ is commutable with $T_n(x)$ then $p_n(x) = T_n(x)$.

Exercise 2.3. Prove that the coefficient on the x^n term of the Chebyshev polynomial is 2^{n-1} . Hint: $(1+x)^n = \sum_{j=0}^n \binom{n}{j} x^j$ for $n > 0$, n a positive integer.

Exercise 2.4. Show that $\sum_{x=1}^n x^3 = \frac{n^2(n+1)^2}{4}$

3. Differentiation of Chebyshev Polynomials

This section will illustrate some of the derivations and applications of the derivatives of Chebyshev polynomials. One of the most important applications is in approximating a function. We will then proceed to take derivatives of the functions and show recurrence relationships between the coefficients of the functions and its derivatives. This last step is important in the application of spectral methods.

3.1. Sturm-Liouville solution and Orthogonality

Chebyshev polynomials can also be defined as the function which satisfies the following differential equation.

$$(1-x^2) \frac{d^2 y}{dx^2} - x \frac{dy}{dx} + n^2 y = 0 \quad (3.1)$$

Since (3.1) is a Sturm-Liouville problem, the Chebyshev polynomial is a particular hypergeometric function.

Chebyshev polynomials are orthogonal functions with respect to a weighting function of $(1-x^2)^{-\frac{1}{2}}$.

$$\int_{-1}^1 T_n(x) T_m(x) (1-x^2)^{-\frac{1}{2}} dx = \frac{\pi}{2} c_n \delta_{nm} \quad (3.2)$$

where

$$c_n = \begin{cases} 2 & n = 0 \\ 1 & n > 0 \end{cases} \quad (3.3)$$

$$\delta_{nm} = \begin{cases} 0 & n \neq m \\ 1 & n = m \end{cases} \quad (3.4)$$

Orthogonality in combination with its geometric rate of convergence are the reasons why this function is so useful.

3.2. Recurrence Relations

Let's say we wanted to approximate a function by a finite series of Chebyshev polynomials.

$$u(x) \simeq u_N(x) = \sum_{n=0}^N a_n T_n(x) \quad (3.5)$$

say we also wanted to approximate the derivatives of the function.

$$u'_N(x) = \sum_{n=0}^{N-1} a_n^{(1)} T_n(x) \quad (3.6)$$

The derivative of u is related to N Chebyshev polynomials by a separate set of coefficients $a_n^{(1)}$. By taking the derivative of (3.5) we obtain.

$$u'_N(x) = \sum_{n=1}^N a_n T'_n(x) \quad (3.7)$$

Note that now the summation begins with $n = 1$ and not $n = 0$, while the summation of (3.6) starts at $n = 0$.

A relationship between a_n and $a_n^{(1)}$ can be found. To prove this, we will make use of the following trigonometric identity.

$$\begin{aligned} 2 \sin r\theta \cos p\theta &= \sin(p+r)\theta - \sin(p-r)\theta \\ 2 \cos p\theta &= \frac{\sin(p+r)\theta}{\sin r\theta} - \frac{\sin(p-r)\theta}{\sin r\theta} \end{aligned} \quad (3.8)$$

Now let $p = n$ and $r = 1$

$$2 \cos n\theta = \frac{\sin(n+1)\theta}{\sin \theta} - \frac{\sin(n-1)\theta}{\sin \theta}$$

which upon substitution of the definition of $T_n(x)$ and $T'_n(x)$ gives.

$$2T_n(x) = \frac{T'_{n+1}(x)}{n+1} - \frac{T'_{n-1}(x)}{n-1} \quad (3.9)$$

Substituting (3.9) into (3.6) and equating it to (3.7) yields.

$$\sum_{n=0}^{N-1} a_n^{(1)} \frac{1}{2} \left[\frac{T'_{n+1}(x)}{n+1} - \frac{T'_{n-1}(x)}{n-1} \right] = \sum_{n=1}^N a_n T'_n(x) \quad (3.10)$$

With the knowledge that $T'_{-m}(x) = T'_m(x)$, we can start writing out terms of (3.10).

$$\begin{aligned} a_0^{(1)} \left[\frac{T'_1(x)}{1} - \frac{T'_{-1}(x)}{-1} \right] + \sum_{n=1}^N a_n^{(1)} \left[\frac{T'_{n+1}(x)}{n+1} - \frac{T'_{n-1}(x)}{n-1} \right] \\ = 2 \sum_{n=1}^N a_n T'_n(x) \end{aligned} \quad (3.11)$$

$$\begin{aligned} 2a_0^{(1)} T'_1(x) + a_1^{(1)} \left[\frac{T'_2(x)}{2} - \frac{T'_0(x)}{0} \right] + a_2^{(1)} \left[\frac{T'_3(x)}{3} - \frac{T'_1(x)}{1} \right] \\ + a_3^{(1)} \left[\frac{T'_4(x)}{4} - \frac{T'_2(x)}{2} \right] + \dots = 2a_1 T'_1 + a_2 T'_2(x) + 2a_3 T'_3(x) + \dots \end{aligned} \quad (3.12)$$

Since $\{T_n(x) : n = 1, 2, \dots, N\}$ make up the basis of an N dimensional Chebyshev space, the coefficients on each term can be set equal to each other. Also note that

$$\lim_{m \rightarrow 0} \frac{T'_m(x)}{m} = \lim_{m \rightarrow 0} \frac{\sin m\theta}{\sin \theta} = \frac{0}{\sin \theta} = 0 \quad (3.13)$$

$$\begin{aligned} 2a_0^{(1)} - a_2^{(1)} &= 2a_1 \\ \frac{a_1^{(1)}}{2} - \frac{a_3^{(1)}}{2} &= 2a_2 \\ \frac{a_2^{(1)}}{3} - \frac{a_4^{(1)}}{3} &= 2a_3 \\ &\vdots \\ a_k^{(1)} - a_{k+2}^{(1)} &= 2(k+1)a_{k+1} \end{aligned} \quad (3.14)$$

in general

$$2ka_k = c_{k-1}a_{k-1}^{(1)} - a_{k+1}^{(1)} \quad \text{for } 1 \leq k \leq N \quad (3.15)$$

where c_k is defined in (3.3)

The same relationship can be developed for the $(q-1)^{th}$ derivative of (3.9).

$$2T_n^{(q-1)}(x) = \frac{T_{n+1}^{(q)}(x)}{n+1} - \frac{T_{n-1}^{(q)}(x)}{n-1} \quad n \geq q \quad (3.16)$$

where $T_n^{(q)}(x)$ is the q^{th} derivative of $T_n(x)$. Applying the same procedure to (3.16) would yield

$$c_k a_k^{(q)} - a_{k+2}^{(q)} = 2(k+1)a_{k+1}^{(q-1)} \quad 0 \leq k \leq N-q \quad (3.17)$$

Starting with (3.14) a simplified form of the recurrence relation can be developed. Notice that $a_k = 0$ for $k \geq N$. Start with $k = N - 1$ and work in descending order.

$$\begin{aligned}
c_{N-1}a_{N-1}^{(1)} - a_{N+1}^{(1)} &= 2(N) a_N \\
c_{N-2}a_{N-2}^{(1)} - a_N^{(1)} &= 2(N-1) a_{N-1} \\
c_{N-3}a_{N-3}^{(1)} - a_{N-1}^{(1)} &= 2(N-2) a_{N-2} \\
&\vdots \\
c_2a_2^{(1)} - a_4^{(1)} &= 2(3) a_3 \\
c_1a_1^{(1)} - a_3^{(1)} &= 2(2) a_2 \\
c_0a_0^{(1)} - a_2^{(1)} &= 2(1) a_2
\end{aligned} \tag{3.18}$$

Simplifying and substituting yields

$$\begin{aligned}
a_{N-1}^{(1)} &= 2(N) a_N \\
a_{N-2}^{(1)} &= 2(N-1) a_{N-1} \\
a_{N-3}^{(1)} - 2(N) a_N &= 2(N-2) a_{N-2} \\
a_{N-4}^{(1)} - 2(N-1) a_{N-1} &= 2(N-3) a_{N-3} \\
&\vdots \\
a_1^{(1)} &= 2 \cdot 2a_2 + 2 \cdot 4a_4 + \cdots + 2(N-1) a_{N-1} \\
c_0a_0^{(1)} &= 2 \cdot 2a_1 + 2 \cdot 4a_3 + \cdots + 2(N) a_N
\end{aligned} \tag{3.19}$$

Put (3.19) into summation form.

$$c_n a_n^{(1)} = 2 \sum_{\substack{p=n+1 \\ p+n \text{ odd}}}^N p a_p \tag{3.20}$$

The relationship between the q^{th} and the $q^{\text{th}} - 1$ derivative coefficients can also be written. In addition (3.20) does not need to be truncated to N terms. The combination of the two gives.

$$c_n a_n^{(q)} = 2 \sum_{\substack{p=n+1 \\ p+n \text{ odd}}}^{\infty} p a_p^{(q-1)} \tag{3.21}$$

To carry this exercise further, let's say we were interested (which we are) in the second derivative recurrence relation between a_n and $a_n^{(2)}$. Let $q = 2$ in (3.21) and substitute (3.20) in for $a_p^{(1)}$.

$$c_n a_n^{(2)} = 2 \sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{\infty} m \left[\frac{2}{c_m} \sum_{\substack{p=m+1 \\ p+m \text{ odd}}}^{\infty} p a_p \right] \quad (3.22)$$

Since m will always be greater than zero, $c_m = 1$. Simplifying (3.22) gives

$$c_n a_n^{(2)} = 4 \sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{\infty} m \left[\sum_{\substack{p=m+1 \\ p+m \text{ odd}}}^{\infty} p a_p \right] \quad (3.23)$$

To get rid of the ∞ in the inner summation we can switch the order of summation. Note that the summations can only be switched when the summations are uniformly convergent. Start by expanding the inner summation.

$$c_n a_n^{(2)} = 4 \sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{\infty} m [(m+1) a_{m+1} + (m+3) a_{m+3} + \dots] \quad (3.24)$$

Followed by the expansion of the outer summation.

$$\begin{aligned} \frac{1}{4} c_n a_n^{(2)} &= (n+1) [(n+2) a_{n+2} + (n+4) a_{n+4} + (n+6) a_{n+6} + \dots] \\ &\quad + (n+3) [(n+4) a_{n+4} + (n+6) a_{n+6} + \dots] \\ &\quad + (n+5) [(n+6) a_{n+6} + (n+8) a_{n+8} + \dots] \\ &\quad \vdots \\ &\quad + (n+2i-1) [(n+2i) a_{n+2i} + (n+2i+2) a_{n+2i+2} + \dots] \end{aligned} \quad (3.25)$$

Regroup the a_i terms and their corresponding coefficients.

$$\begin{aligned} &4 \{ (n+2) a_{n+2} [n+1] \\ &\quad + (n+4) a_{n+4} [(n+1) + (n+3)] \\ &\quad + (n+6) a_{n+6} [(n+1) + (n+3) + (n+5)] \\ &\quad \vdots \\ &\quad + (n+2i) a_{n+2i} [(n+1) + (n+3) + \dots + (n+2i-1)] \} \\ &\quad \vdots \end{aligned} \quad (3.26)$$

Write the inside brackets as a summation.

$$4(n+2i)a_{n+2i} \sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{n+2i-1} m \quad \text{for } i = 1, 2, 3, \dots \quad (3.27)$$

and finally

$$c_n a_n^{(2)} = 4 \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^{\infty} p a_p \sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{p-1} m \quad (3.28)$$

Recalling from section 2.5 on the methods of summation, we saw ways of finding the value of $\sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{p-1} m$. It would be more aesthetic and computational less intensive if there existed a single value that would replace this summation. Begin by expanding the summation.

$$\sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{p-1} m = (n+1) + (n+3) + \dots + (p-1) \quad (3.29)$$

$$= \sum_{x=1}^{\frac{p-n}{2}} n + (2x-1) = \sum_{x=1}^{\frac{p-n}{2}} (n-1) + 2 \sum_{x=1}^{\frac{p-n}{2}} x \quad (3.30)$$

Let $k = \frac{p-n}{2}$. Look at first of the two summations on the right hand side of (3.30).

$$\sum_{x=1}^k (n-1) = (n-1) \sum_{x=1}^k \Delta x^{(1)} = (n-1) x \Big|_{x=1}^{x=k+1} = (n-1)k \quad (3.31)$$

Now look at the second summation of (3.30).

$$2 \sum_{x=1}^k x = 2 \sum_{x=1}^k \Delta \frac{x^{(2)}}{2} = x^{(2)} \Big|_{x=1}^{x=k+1} = (k+1)k \quad (3.32)$$

$$\begin{aligned} \sum_{\substack{m=n+1 \\ m+n \text{ odd}}}^{p-1} m &= (n-1)k + (k+1)k \quad (3.33) \\ &= k[(n-1) + (k+1)] = k(n+k) \\ &= \left(\frac{p-n}{2}\right) \left(n + \frac{p-n}{2}\right) = \frac{1}{4}(p^2 - n^2) \end{aligned}$$

Substituting back into (3.28) and truncating to N terms gives.

$$c_n a_n^{(2)} = \sum_{\substack{p=n+2 \\ p+n \text{ even}}}^N p(p^2 - n^2) a_p \quad (3.34)$$

Equation (3.34) is a convenient way of representing the second derivative of a function in terms of a series of Chebyshev polynomials.

There is another formula which is very important in solving boundary value problems. The equation gives the value of the p^{th} order derivative of a Chebyshev polynomial when evaluated at one of its end points, 1 or -1 .

$$\frac{d^p}{dx^p} T_n(\pm 1) = (\pm 1)^{n+p} \prod_{k=0}^{p-1} \frac{(n^2 - k^2)}{(2k + 1)} \quad (3.35)$$

Equation (3.35) is given without proof but has been verified by the author in several problems. Notice that instead of using coefficients to relate the derivative of the function to the zeroth order derivative of the Chebyshev polynomial, one directly takes the derivative of the Chebyshev polynomial and then evaluates it at the end points. Equation (3.35) gives an extremely useful method for evaluating derivatives in boundary conditions.

3.3. Matrix Notation

In the last section, summation notation was used to develop recurrence relationships between expansion coefficients of a function (i.e. a_n) and the expansion coefficients of derivatives of the function (i.e. $a_n^{(1)}$). In this section, a matrix notation will be used to develop the same relationship between a_n and $a_n^{(1)}$ as well as other expansion coefficients. In my personal experience this method proved the most insightful and easiest to derive. It does not, however, deal very well with recurrence relationships such as the following expansion.

$$x u_N(x) = \sum_{n=0}^{\infty} b_n T_n(x) \quad (3.36)$$

or

$$x u'_N(x) = \sum_{n=0}^{\infty} b_n^{(1)} T_n(x) \quad (3.37)$$

The matrix notation will be used in the next section which explores the application of Chebyshev Polynomials to spectral methods.

Look back at the recurrence equation (3.18). Put the equations into matrix form by letting $\mathbf{a} = (a_0^{(1)}, a_1^{(1)}, \dots, a_{N-1}^{(1)})^T$ and remembering that $c_0 = 2$, $c_n = 1$ for $n \geq 0$.

$$\begin{pmatrix} 2 & 0 & -1 & 0 & \cdots & 0 \\ 0 & 1 & 0 & -1 & \cdots & 0 \\ 0 & 0 & 1 & 0 & & 0 \\ \vdots & & & \ddots & \ddots & \vdots \\ \vdots & & & & & 1 & 0 \\ 0 & \cdots & \cdots & \cdots & 0 & 1 \end{pmatrix} \begin{pmatrix} a_0^{(1)} \\ a_1^{(1)} \\ \vdots \\ \vdots \\ a_{N-1}^{(1)} \end{pmatrix} = \begin{pmatrix} 0 & 2 & 0 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 4 & 0 & \cdots & \cdots & 0 \\ 0 & 0 & 0 & 6 & \ddots & & 0 \\ \vdots & & & \ddots & \ddots & & \vdots \\ \vdots & & & & & 2(N-1) & \\ 0 & \cdots & \cdots & \cdots & \cdots & 0 & 2N \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ \vdots \\ a_{N-1} \\ a_N \end{pmatrix} \quad (3.38)$$

which can be written in matrix form as

$$\mathbf{C} \cdot \mathbf{a}^{(1)} = \mathbf{A} \cdot \mathbf{a} \quad (3.39)$$

Since \mathbf{C} is an upper triangular matrix, $\det(\mathbf{C})$ is the product of its diagonal entries which here $\det(\mathbf{C}) = 2$. As $\det(\mathbf{C}) \neq 0$, \mathbf{C} is non-singular and \mathbf{C}^{-1} exists. This allows (3.38) to be multiplied by \mathbf{C}^{-1} .

$$\mathbf{a}^{(1)} = \mathbf{C}^{-1} \cdot \mathbf{A} \cdot \mathbf{a} \quad (3.40)$$

Let $\mathbf{C}^{-1} \cdot \mathbf{A} = \mathbf{E}$. This gives $\mathbf{a}^{(1)} = \mathbf{E} \cdot \mathbf{a}$. In general the expression for the q^{th} derivative can be written

$$\mathbf{a}^{(q)} = \mathbf{E} \cdot \mathbf{a}^{(q-1)} \quad (3.41)$$

$$\mathbf{a}^{(2)} = \mathbf{E} \cdot \mathbf{a}^{(1)} = \mathbf{E} \cdot \mathbf{E} \cdot \mathbf{a} = \mathbf{E}^2 \cdot \mathbf{a} \quad (3.42)$$

in general we have

$$\mathbf{a}^{(k)} = \mathbf{E}^k \cdot \mathbf{a} \quad (3.43)$$

where $\mathbf{E}^k = \underbrace{\mathbf{E} \cdot \mathbf{E} \cdot \mathbf{E} \cdots \mathbf{E}}_{k \text{ times}}$

It can be shown that

$$\mathbf{E} = \begin{pmatrix} 0 & 1 & 0 & 3 & 0 & 5 & 0 & 7 & 0 & \dots & 2N \\ 0 & 0 & 4 & 0 & 8 & 0 & 12 & 0 & 0 & & 0 \\ 0 & 0 & 0 & 6 & 0 & 10 & 0 & 14 & 0 & \dots & 2N \\ \vdots & & & & & & & \ddots & \ddots & & \\ 0 & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & 2N \\ 0 & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & \dots & 0 \end{pmatrix} \quad (3.44)$$

which corresponds with

$$\mathbf{E} = [\mathbf{E}_{(n+1)(m+1)}] = \frac{2}{c_n} m \quad \text{for} \quad \begin{array}{l} n = 0, 1, \dots, N-2 \\ m = n+1, n+3, \dots, N \end{array} \quad (3.45)$$

and that

$$\mathbf{E}^2 = \begin{pmatrix} 0 & 0 & 4 & 0 & 32 & 0 & 108 & 0 & 256 & \dots & \dots \\ 0 & 0 & 0 & 24 & 0 & 120 & 0 & 336 & 0 & & \vdots \\ 0 & 0 & 0 & 0 & 48 & 0 & 192 & 0 & 480 & & \vdots \\ \vdots & & & & & 80 & 0 & 280 & 0 & & \vdots \\ \vdots & & & & & & 120 & 0 & 384 & \ddots & \vdots \\ 0 & \dots & \dots & \dots & \dots & \dots & & \ddots & \ddots & \ddots & \vdots \\ 0 & \dots & \dots & \dots & \dots & \dots & & & \dots & \dots & 0 \\ 0 & \dots & \dots & \dots & \dots & \dots & & & \dots & \dots & 0 \end{pmatrix} \quad (3.46)$$

which corresponds with

$$\mathbf{E} = [\mathbf{E}_{(n+1)(p+1)}] = \frac{1}{c_n} p (p^2 - n^2) \quad \begin{array}{l} n = 0, 1, 2, \dots, N-3 \\ p = n+2, n+4, \dots, N \end{array} \quad (3.47)$$

The main focus of this section was to take a function and derivatives of that function, which we wanted to expand into Chebyshev Polynomials, and show that the expansion coefficients of each can be related. This was done by two methods, summation notation and matrix notation. The matrix notation is useful in demonstrating how to solve for systems of differential equations. It will also be used to solve for a variety of eigenvalue problems. The recurrence relationships are preferred when only the solution vector to a problem is desired. Most of the common recurrence relationships for linear operators are tabulated in the appendix of Gottlieb and Orszag's book, *Numerical Analysis of Spectral Methods* [4].

3.4. Problems

Exercise 3.1. Prove that $T_n(x) = \cos n\theta$ is the solution to

$$(1-x^2) \frac{d^2 T_n(x)}{dx^2} - x \frac{dT_n(x)}{dx} + n^2 T_n(x) = 0$$

Exercise 3.2. Prove that

$$\int_{-1}^1 T_n(x) T_m(x) (1-x^2)^{-\frac{1}{2}} dx = \frac{\pi}{2} c_n \delta_{nm}$$

Exercise 3.3. If $\phi_r(x)$ is a real orthogonal function with respect to a weighting function $w(x)$ and $w(x) > 0$ on the interval $\mathcal{I} = -1 \leq x \leq 1$. Prove that $\phi_r(x)$ has r real and distinct roots on the interval \mathcal{I} .

Exercise 3.4. Prove

$$c_n a_n^{(3)} = \frac{1}{4} \sum_{\substack{m=n+3 \\ m+n \text{ odd}}}^N m [(m-n)^2 - 1] [(m+n)^2 - 1] a_m \quad (3.48)$$

Exercise 3.5. Prove

$$c_n a_n^{(4)} = \frac{1}{24} \sum_{\substack{p=n+4 \\ p+n \text{ even}}}^N p \left[p^2 (p^2 - 4)^2 - 3n^2 p^4 + 3n^4 p^2 - n^2 (n^2 - 4)^2 \right] a_p \quad (3.49)$$

Exercise 3.6. Prove that the derivative of $T_n(x)$ evaluated at the boundary of its interval is

$$\frac{d}{dx} T_n(\pm 1) = (-1)^{n+1} n^2$$

4. Spectral Tau Methods

4.1. Introduction

Spectral Methods are a particular numerical scheme for solving differential equations. It is a discretization scheme developed from the Method of Weighted Residuals (MWR) [1]. The Tau method is one of the three most commonly used techniques of spectral methods. The three techniques are Galerkin, collocation and tau. This section will concentrate solely on the tau method. The interested reader

is referred to *Spectral Methods in Fluid Dynamics* [2] for examples of the other two methods.

Before further explanation of the spectral tau method, a brief review of the method of weighted residuals may be appropriate. Given the problem

$$\frac{\partial u}{\partial t} = \mathbf{L}u + f \quad (4.1)$$

$$\mathbf{B}u = 0 \quad (4.2)$$

where \mathbf{L} is some linear spatial operator and \mathbf{B} is a linear boundary operator. We want to express $u(x, t)$ as an infinite sum of some trial function $\phi_n(x)$.

$$u(x, t) = \sum_{n=1}^{\infty} a_n(t) \phi_n(x) \quad (4.3)$$

the function is then approximated by truncating the series to N terms.

$$u_N(x, t) = \sum_{n=1}^N a_n(t) \phi_n(x) \quad (4.4)$$

Now choose a test function $\psi_m(x)$ such that $\phi_n(x)$ is orthonormal to $\psi_m(x)$ on some interval $\mathcal{I} = a \leq x \leq b$ for a given inner product $\langle *, * \rangle$.

$$\langle \phi_n(x), \psi_m(x) \rangle = \int_a^b \phi_n(x) \overline{\psi_m(x)} dx = \delta_{nm} \quad (4.5)$$

where $\overline{\psi_m(x)}$ is the complex conjugate of $\psi_m(x)$. The essence of the Galerkin method is to find the set $\{a_n(t) : n = 1, 2, \dots, N\}$ such that the errors $\{\epsilon_n\}$ are minimized. The error is defined as

$$\frac{\partial u}{\partial t} - \frac{\partial u_N}{\partial t} - \mathbf{L}u + \mathbf{L}u_N - f + f_N = \epsilon_n$$

To find the set of coefficients $\{a_n(t) : n = 1, 2, \dots, N\}$ multiply both sides of the governing equation (4.1) by the test function and take the inner product $\langle *, * \rangle$ such that

$$\frac{\partial}{\partial t} \langle \psi_m(x), u_N \rangle = \langle \psi_m(x), \mathbf{L}u_N \rangle + \langle \psi_m(x), f \rangle \quad (4.6)$$

$$\sum_{n=1}^N \langle \psi_m(x), \phi_n(x) \rangle \frac{d\overline{a_m}}{dt} = \sum_{n=1}^N \overline{a_m} \langle \psi_m(x), \mathbf{L}\phi_n(x) \rangle + \langle \psi_m(x), f \rangle \quad (4.7)$$

Take the complex conjugate of the equation and note that $\langle \psi_m, \phi_n \rangle = \delta_{nm}$. This yields

$$\frac{da_m}{dt} = \sum_{n=1}^N a_n \langle \psi_m(x), \mathbf{L}\phi_n(x) \rangle + \langle f, \psi_m(x) \rangle \quad (4.8)$$

Equation (4.8) can be solved by well known methods which will depend upon the operator \mathbf{L} and the inner product.

4.2. Spectral Tau Methods

Notice that the choice of the trial function $\phi_n(x)$ must satisfy the essential boundary conditions. For particular problems, the boundary conditions can be complicated. Choosing a trial function which satisfies the boundary conditions exactly can become extremely difficult if not impossible. The spectral tau method offers a solution to this problem. The solution is quite simple in its concept. Instead of trying to satisfy the boundary condition by choosing the proper trial function, just add more constants to the expansion.

$$u_N(x, t) = \sum_{n=1}^{N+k} a_n(t) \phi_n(x) \quad (4.9)$$

Here N is the dimension in the domain and k is the number of boundary conditions. So before where $\phi_n(x)$ was forced to satisfy the boundary conditions, we just add k more coefficients, $\{a_n(t) : n = N + 1, \dots, N + k\}$, to be solved. The k additional equations needed are produced from the boundary conditions.

$$\sum_{n=1}^{N+k} a_n \mathbf{B}\phi_n(x) = 0 \quad (4.10)$$

So the complete set of $N + k$ equations to be solved for the set of $N + k$ coefficients are the N equations of (4.8) and the k equations of (4.10).

The application of Chebyshev polynomials to the spectral tau method is to let

$$\phi_n(x) = T_n(x) \quad (4.11)$$

and

$$\psi_m(x) = \frac{2}{\pi c_m} T_m(x) (1 - x^2)^{-\frac{1}{2}} \quad (4.12)$$

The best way to explain the use of Chebyshev spectral tau method is to work out an example.

Example 4.1. *The following system is a second order differential equation with homogeneous boundary conditions.*

$$\frac{d^2u}{dx^2} = 1 \quad (4.13)$$

$$u(-1) = 0 \quad (4.14)$$

$$\frac{du(1)}{dx} = 0 \quad (4.15)$$

Solve for u using the Chebyshev spectral tau method. This system has the solution $u(x) = \frac{1}{2}x^2 - x - \frac{3}{2}$.

First apply

$$u(x) = \sum_{n=0}^N a_n T_n(x) \quad (4.16)$$

Here the order of the summation has been changed to $n = 0$ to $n = N$. We will need the first and second order derivatives of $u(x)$ as they relate to $T_n(x)$. For this, equations (3.20) and (3.34) will be used.

$$\frac{du}{dx} = \sum_{n=0}^{N-1} a_n^{(1)} T_n(x) \quad (4.17)$$

$$\frac{d^2u}{dx^2} = \sum_{n=0}^{N-2} a_n^{(2)} T_n(x) \quad (4.18)$$

Substitute (4.16) into the governing equation (4.13) and the boundary conditions (4.14) and (4.15).

$$\sum_{n=0}^{N-2} a_n^{(2)} T_n(x) = 1 \quad (4.19)$$

$$\sum_{n=0}^N a_n T_n(-1) = 0 \quad (4.20)$$

$$\sum_{n=0}^{N-1} a_n^{(1)} T_n(1) = 0 \quad (4.21)$$

Alternatively and preferentially, we can use equation (3.35) for (4.21). Equation (3.35) is preferred because it is easier to program in FORTRAN. When (3.35)

is used on the boundaries, the lower index must be raised to the order of the derivative. So in general,

$$\frac{d^p u_N}{dx^p} = \sum_{n=p}^N a_n \frac{d^p T_n'(x)}{dx^p} \quad (4.22)$$

For this problem we will use the recurrence relationship of $a_n^{(1)}$. In the next and subsequent problems, (3.35) will be used. As an exercise, the reader should use both methods to verify that each will obtain the same result. So (4.21) can be written as

$$\sum_{n=1}^N a_n T_n'(1) = \sum_{n=1}^N a_n n^2 \quad (4.23)$$

The first step will be to take the inner product of the domain equation (4.19)

$$\sum_{n=0}^{N-2} a_n^{(2)} \langle T_n(x), \psi_m(x) \rangle = \langle 1, \psi_m(x) \rangle = \langle T_0(x), \psi_m(x) \rangle \quad (4.24)$$

where

$$\langle T_n(x), \psi_m(x) \rangle = \frac{2}{\pi c_n} \int_{-1}^1 T_n(x) T_m(x) (1-x^2)^{-\frac{1}{2}} dx = \delta_{nm} \quad (4.25)$$

this gives.

$$a_n^{(2)} = \delta_{0n} = \begin{cases} 1 & n = 0 \\ 0 & 0 < n \leq N - 2 \end{cases} \quad (4.26)$$

On the boundaries, we need only evaluate the Chebyshev polynomials, $T_n(1) = 1$ and $T_n(-1) = (-1)^n$. Upon substitution into (4.20) and (4.23) yields

$$\sum_{n=0}^N a_n (-1)^n = 0 \quad (4.27)$$

$$\sum_{n=1}^N n^2 a_n = 0 \quad (4.28)$$

This gives $N + 1$ equations, $N - 1$ for (4.26) plus the two boundary equations (4.27) and (4.28). Let $N = 5$ and write out equation (4.26) using the recurrence relationship for the second derivative expansion coefficient from equation (3.34).

$$a_0^{(2)} = \frac{1}{2} [2 \cdot 4a_2 + 4 \cdot 16a_4] = 1$$

$$\begin{aligned}
a_1^{(2)} &= 3 \cdot (9 - 1) a_3 + 5 \cdot (25 - 1) a_5 = 0 \\
a_2^{(2)} &= 4 \cdot (16 - 4) a_4 = 0 \\
a_3^{(2)} &= 5 \cdot (25 - 9) a_5 = 0
\end{aligned} \tag{4.29}$$

The boundary conditions are

$$a_0 - a_1 + a_2 - a_3 + a_4 - a_5 = 0 \tag{4.30}$$

$$a_1 + 4a_2 + 9a_3 + 16a_4 + 25a_5 = 0 \tag{4.31}$$

Put the $N + 2$ equations into matrix form.

$$\begin{pmatrix} 0 & 0 & 4 & 0 & 32 & 0 \\ 0 & 0 & 0 & 24 & 0 & 120 \\ 0 & 0 & 0 & 0 & 48 & 0 \\ 0 & 0 & 0 & 0 & 0 & 80 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 0 & 1 & 4 & 9 & 16 & 25 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \\ a_4 \\ a_5 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \tag{4.32}$$

The solution to (4.32) is $\mathbf{a} = \left(-\frac{5}{4}, -1, \frac{1}{4}, 0, 0, 0\right)^{\mathbf{T}}$, substitute into (4.16).

$$\begin{aligned}
u_N(x) &= -\frac{5}{4}T_0(x) - T_1(x) + \frac{1}{4}T_2(x) \\
&= -\frac{5}{4} - x + \frac{1}{4}(2x^2 - 1) = \frac{1}{2}x^2 - x - \frac{3}{2}
\end{aligned}$$

which is the exact solution.

The matrix notation is a heuristic lesson in solving differential equations with the spectral method. The matrix notation is also an excellent way of solving for eigenvalue problems. When only the solution vector is needed, the use of the recurrence relation (3.17) is preferred. The reason is purely computational. In general, solving eigenvalue problems take of order N^3 operations. The recurrence relation will usually form a tridiagonal system (for one dimensional problems) which can be solved with much more efficient algorithms [12]. An example of how this is done is given in *Spectral Methods in Fluid Dynamics* pp. 129-131 [2].

Now we will demonstrate the use of Chebyshev spectral tau methods in solving eigenvalue problems.

Example 4.2. *This example deals with an eigenvalue problem with homogeneous boundary conditions. We will try to solve for the first few eigenvalues, λ .*

$$\frac{d^2u}{dy^2} + \lambda^2u = 0 \quad (4.33)$$

$$u|_{y=0} = 0 \quad (4.34)$$

$$\left. \frac{du}{dy} \right|_{y=1} + u \Big|_{y=1} = 0 \quad (4.35)$$

The analytical solution for λ is

$$\lambda = -\tan \lambda \quad (4.36)$$

In this example, we will more closely look at the details of each step. This careful analysis will shed light on some of the intricacies involved in this method. There are three key steps that must be applied between the system of equations, which comprise of the governing equations and the boundary conditions, and the set of equations that need to be solved for the expansion coefficients, a_n . The first step is to interpolate or approximate the function $u(x)$ into Chebyshev space.

$$u(x) \simeq u_N(x) = \sum_{n=0}^N a_n T_n(x) \quad (4.37)$$

The interpolated function, $u_N(x)$, is projected into the equation space. This step will be explained in more detail later. And finally, take the inner product of the domain equations (governing equation) and evaluate the projected functions on the boundaries.

Notice that the Chebyshev polynomials lie in the interval of $-1 \leq x \leq 1$ and the problem is stated on the interval of $0 \leq y \leq 1$. In order to transform the problem into the proper space, we will apply a stretching function (more commonly called a coordinate transformation). The stretching function we need here is $x = 2y - 1$. Transforming the system of equations (4.33) through (4.35) yields.

$$\left(\frac{dx}{dy} \right)^2 \frac{d^2u}{dx^2} + \lambda^2u = 0 \quad (4.38)$$

$$u|_{x=-1} = 0 \quad (4.39)$$

$$\left(\frac{dx}{dy} \right) \left. \frac{du}{dx} \right|_{x=1} + u \Big|_{x=1} = 0 \quad (4.40)$$

Using the derivative $\frac{dx}{dy} = 2$ and interpolating $u(x)$ into $u_N(x)$ will give.

$$4 \frac{d^2 u_N}{dx^2} + \lambda^2 u_N = 0 \quad (4.41)$$

$$u_N|_{x=-1} = 0 \quad (4.42)$$

$$2 \left. \frac{du_N}{dx} \right|_{x=1} + u_N \Big|_{x=1} = 0 \quad (4.43)$$

Notice that now the problem is cast into $u_N(x)$, the solution technique will find the exact solution to $u_N(x)$. If $u(x)$ is exactly cast into $u_N(x)$ then the exact solution to $u(x)$ will be found. In general if $u(x)$ is a polynomial of degree equal to or less than the degree of the Chebyshev polynomial being used, then the exact solution to $u(x)$ will be found. That is why example 4.1 came up with the exact solution. In this problem, and in general, we will not find the exact solution, since there exists an infinite number of eigenvalues.

Substitute (4.37) for $u_N(x)$ into (4.41), (4.42) and (4.43).

$$4 \sum_{n=0}^{N-2} a_n^{(2)} T_n(x) + \lambda^2 \sum_{n=0}^N a_n T_n(x) = 0 \quad (4.44)$$

$$\sum_{n=0}^N a_n T_n(-1) = 0 \quad (4.45)$$

$$2 \sum_{n=1}^N n^2 a_n T_n(1) + \sum_{n=0}^N a_n T_n(1) = 0 \quad (4.46)$$

The last key step is to take the inner product of (4.44) and evaluate $T_n(-1)$ and $T_n(1)$ in (4.45) and (4.46), respectively. Remember from the Tau method, that the inner product of (4.44) will be taken $N - 2$ times; N minus the number of boundary conditions. It is important to note that we will subtract from equations in which the boundary conditions apply to. This will become important when there is more than one differential equation.

$$4a_n^{(2)} + \lambda^2 a_n = 0 \quad \text{for } n = 0, 1, \dots, N - 2 \quad (4.47)$$

$$\sum_{n=0}^N a_n (-1)^n = 0 \quad (4.48)$$

$$2 \sum_{n=1}^N n^2 a_n + \sum_{n=0}^N a_n = 0 \quad (4.49)$$

By using the matrix notation developed in the last part of section 3, (4.47) through (4.49) can be simplified.

$$(4\mathbf{E}^2 + \lambda^2\mathbf{I}) \cdot \mathbf{a} = 0 \quad (4.50)$$

$$(-1)^n I \cdot \mathbf{a} = 0 \quad (4.51)$$

$$(2n^2 I + I) \cdot \mathbf{a} = 0 \quad (4.52)$$

where $(-1)^n I = (1, -1, 1, -1, \dots, (-1)^N)$ and $2n^2 I = (0, 2, 8, 18, \dots, 2N^2)$. Note that $4\mathbf{E}^2 + \lambda^2\mathbf{I}$ is an $(N - 1) \times (N + 1)$ matrix. The last two rows needed to make a square matrix come from (4.51) and (4.52). Also notice that the I in (4.51) is a vector with $N + 1$ entries equal to one. This notation leads into the format that will be needed to write a numerical computation.

Now the initial statement of the problem was to find the first few eigenvalues of the system. We can achieve this by rewriting (4.50) through (4.52) as.

$$4\mathbf{E}^2 \cdot \mathbf{a} = -\lambda^2\mathbf{I} \cdot \mathbf{a} \quad (4.53)$$

$$(-1)^n I \cdot \mathbf{a} = 0 \quad (4.54)$$

$$(2n^2 I + I) \cdot \mathbf{a} = 0 \quad (4.55)$$

Equations (4.53) through (4.55) give a generalized eigenvalue problem

$$\mathbf{A} \cdot \mathbf{a} = \omega\mathbf{C} \cdot \mathbf{a} \quad (4.56)$$

where for $N = 5$

$$\mathbf{A} = \begin{pmatrix} 4\mathbf{E}^2 \\ (-1)^n I \\ 2n^2 I + I \end{pmatrix} = \begin{pmatrix} 0 & 0 & 16 & 0 & 128 & 0 \\ 0 & 0 & 0 & 96 & 0 & 480 \\ 0 & 0 & 0 & 0 & 192 & 0 \\ 0 & 0 & 0 & 0 & 0 & 320 \\ 1 & -1 & 1 & -1 & 1 & -1 \\ 1 & 3 & 9 & 19 & 33 & 51 \end{pmatrix} \quad (4.57)$$

$$\mathbf{C} = \begin{pmatrix} -\mathbf{I} \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (4.58)$$

and $\omega = \lambda^2$ is the eigenvalue. Note that both \mathbf{A} and \mathbf{C} are $(N + 1) \times (N + 1)$ matrices. If the matrices \mathbf{A} and \mathbf{C} were imported into a computer program and then subsequently passed to a generalized eigenvalue solver, the first few values of λ can be found.

To calculate the first few eigenvalues, I used MathCad[®] version 5.0+ . A general eigenvalue solver is available in this software. Below is a table of the first four eigenvalues for different values of N and the analytic values of λ found using equation (4.36).

Table 4.1 First four eigenvalues of Example 4.2 for various values of N and the actual value.

N	4	5	6	7	8	9	Actual
λ_1	1.990	2.029	2.029	2.029	2.029	2.029	2.029
λ_2	5.73	4.966	4.917	4.914	4.913	4.913	4.913
λ_3	—	9.377	8.204	8.076	7.981	7.978	7.798
λ_4	—	22.44	13.96	12.30	11.23	11.10	11.09

The next example will illustrate how multiple, connected domains can be solved. The main point to this exercise is to demonstrate how sets of coefficients can be concatenated to form a new larger set. This new set of coefficients can then be solved in the same manner as before.

Example 4.3. *The following system describes the heat conduction between two solids. It is assumed that the heat flux and the temperatures are equal at the interface of the two solids. The temperature is held constant at the outer, exposed surfaces. Solve for the first few eigenvalues.*

$$\frac{d^2u}{dy^2} + \lambda^2u = 0 \quad (4.59)$$

$$\frac{d^2v}{dy^2} + \lambda^2v = 0 \quad (4.60)$$

$$u|_{y=l_1} = 0 \quad (4.61)$$

$$v|_{y=l_2} = 0 \quad (4.62)$$

$$u|_{y=0} = v|_{y=0} \quad (4.63)$$

$$\left. \frac{du}{dy} \right|_{y=0} = \left. \frac{dv}{dy} \right|_{y=0} \quad (4.64)$$

The eigenvalues for this system can be found analytically.

$$\lambda = \left(\frac{n\pi}{l_1 + l_2} \right) \quad \text{for } n = 1, 2, 3, \dots \quad (4.65)$$

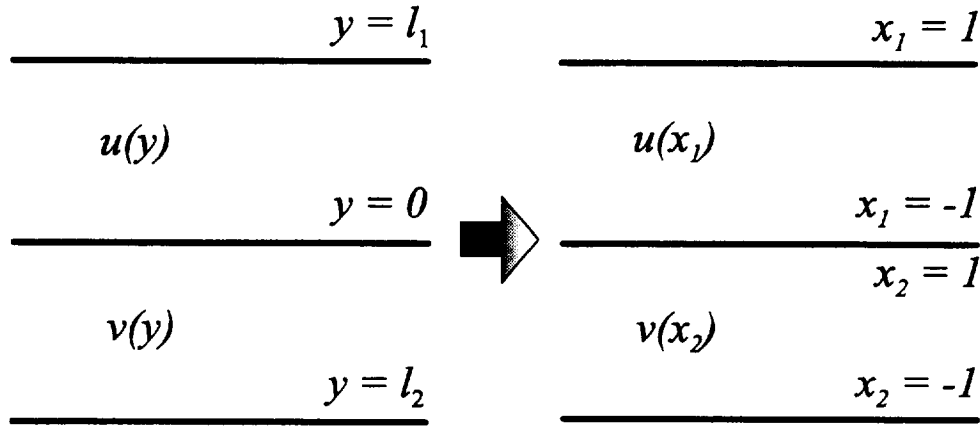


Figure 4.1: Coordinate transformation from y to x_1 and x_2

Figure ?? shows the coordinate transformation that is needed here.

First we will break the two layers up into two different domains. The top layer $0 \leq y \leq l_1$ will be transformed to the first new variable $-1 \leq x_1 \leq 1$ and the bottom layer $l_2 \leq y \leq 0$ will be transformed into the second new variable $-1 \leq x_2 \leq 1$. The coordinate transformation is given in the following two equations.

$$x_1 = \left(\frac{2}{l_1}\right)y - 1 \quad (4.66)$$

$$x_2 = -\left(\frac{2}{l_2}\right)y + 1 \quad (4.67)$$

Apply the coordinate transformation to equations (4.59) through (4.64).

$$\left(\frac{2}{l_1}\right)^2 \frac{d^2u}{dx_1^2} + \lambda^2 u = 0 \quad (4.68)$$

$$\left(\frac{2}{l_2}\right)^2 \frac{d^2v}{dx_2^2} + \lambda^2 v = 0 \quad (4.69)$$

$$u|_{x_1=1} = 0 \quad (4.70)$$

$$v|_{x_2=-1} = 0 \quad (4.71)$$

$$u|_{x_1=-1} = v|_{x_2=1} \quad (4.72)$$

$$\left(\frac{2}{l_1}\right) \frac{du}{dx_1} \Big|_{x_1=-1} = -\left(\frac{2}{l_2}\right) \frac{dv}{dx_2} \Big|_{x_2=1} \quad (4.73)$$

Two separate approximation functions are needed when applying the spectral method to $u(x_1)$ and $v(x_2)$.

$$u_N(x_1) = \sum_{n=0}^N a_n T_n(x_1) \quad \text{for } -1 \leq x_1 \leq 1 \quad (4.74)$$

$$v_M(x_2) = \sum_{m=0}^M b_m T_m(x_2) \quad \text{for } -1 \leq x_2 \leq 1 \quad (4.75)$$

Substitute (4.74) and (4.75) into (4.68) through (4.73) and take the inner product of (4.68) and (4.69).

$$\left(\frac{2}{l_1}\right)^2 a_n^{(2)} + \lambda^2 a_n = 0 \quad \text{for } n = 0, 1, \dots, N-2 \quad (4.76)$$

$$\left(\frac{2}{l_2}\right)^2 b_m^{(2)} + \lambda^2 b_m = 0 \quad \text{for } m = 0, 1, \dots, M-2 \quad (4.77)$$

$$\sum_{n=0}^N a_n = 0 \quad (4.78)$$

$$\sum_{m=0}^M b_m (-1)^m = 0 \quad (4.79)$$

$$\sum_{n=0}^N a_n (-1)^n = \sum_{m=0}^M b_m \quad (4.80)$$

$$\left(\frac{2}{l_1}\right) \sum_{n=1}^N n^2 a_n (-1)^n = -\left(\frac{2}{l_2}\right) \sum_{m=1}^M m^2 b_m \quad (4.81)$$

If we tried to apply the matrix notation, we will run into some difficulties. The dependence of a_n on b_m and vice versa, creates difficulties in setting up the problem to be solved numerically. One way to work around this is to concatenate the set $\{a_n : n = 0, 1, \dots, N\}$ with the set $\{b_m : m = 0, 1, \dots, M\}$ to create a new set, call it $\{c_p : p = 0, 1, \dots, P\}$. Now use the new set in (4.76) through (4.81) and

apply the matrix notation.

$$\begin{pmatrix} \left(\frac{2}{l_1}\right)^2 \mathbf{E}^2 & \mathbf{0} \\ \mathbf{0} & \left(\frac{2}{l_2}\right)^2 \mathbf{E}^2 \\ I & 0 \\ 0 & (-1)^{p-N-1} I \\ (-1)^n I & -I \\ (-1)^n \left(\frac{l_2}{l_1}\right) n^2 I & (p-N-1)^2 I \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ \vdots \\ c_{P-1} \\ c_P \end{pmatrix} = \lambda^2 \begin{pmatrix} -\mathbf{I} & \mathbf{0} \\ \mathbf{0} & -\mathbf{I} \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \\ 0 & 0 \end{pmatrix} \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ \vdots \\ c_{P-1} \\ c_P \end{pmatrix} \quad (4.82)$$

The first row in the left and right hand side matrix of (4.82) actually has $N - 1$ rows, as well as the second row. The last four rows are exactly four rows. The first column is N large and the second column is M large. To clarify the appearance of (4.82), let $N = 4$ and $M = 4$. This gives $P = 9$, which maps as follows, $\{a_n : n = 0, 1, \dots, 4\} = \{c_p : p = 0, 1, \dots, 4\}$ and $\{b_m : m = 0, 1, \dots, 4\} = \{c_p : p = 5, 7, \dots, 9\}$. Substitute in the values of \mathbf{E}^2 and I , and explicitly write out the left hand side matrix of (4.82).

$$\begin{pmatrix} 0 & 0 & 4\left(\frac{2}{l_1}\right)^2 & 0 & 32\left(\frac{2}{l_1}\right)^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 24\left(\frac{2}{l_1}\right)^2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 48\left(\frac{2}{l_1}\right)^2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 4\left(\frac{2}{l_2}\right)^2 & 0 & 32\left(\frac{2}{l_2}\right)^2 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 24\left(\frac{2}{l_2}\right)^2 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 48\left(\frac{2}{l_2}\right)^2 \\ 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 & -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 & 1 & -1 & -1 & -1 & -1 & -1 \\ 0 & \left(\frac{l_2}{l_1}\right) 1 & -4\left(\frac{l_2}{l_1}\right) & 9\left(\frac{l_2}{l_1}\right) & -16\left(\frac{l_2}{l_1}\right) & 0 & 1 & 4 & 9 & 16 \end{pmatrix} \quad (4.83)$$

The right hand side matrix of (4.82) looks like

$$\begin{pmatrix} -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \end{pmatrix} \quad (4.84)$$

Again, if the two matrices were imported into a computer program, a generalized eigenvalue solver could find the eigenvalues, λ , as well as the solution of coefficients, $\{c_p : p = 0, 1, \dots, P\}$.

The following example will show how Chebyshev spectral methods can be used to solve for eigenvalue problems where the eigenvalue is located in the boundary condition. The example is a heat transfer model in a semi-infinite slab. The temperature is held constant at the bottom of the slab and there is Newtonian cooling at the top of the slab. The cooling rate is determined by the heat transfer coefficient, h .

Example 4.4. *Solve for the heat transfer coefficient, h , which will not give a trivial solution to the problem using Chebyshev spectral tau methods. The analytical solution to h is $-\lambda \cot(\lambda)$.*

$$\frac{d^2u}{dx^2} + \lambda^2u = 0 \quad (4.85)$$

$$\frac{du}{dx} + hu = 0 \quad \text{at } x = 1 \quad (4.86)$$

$$u = 0 \quad \text{at } x = -1 \quad (4.87)$$

Here λ is fixed and h is the eigenvalue we wish to solve for. Again we will substitute the Chebyshev series in for u .

$$u = \sum_{n=0}^N a_n T_n(x) \quad (4.88)$$

$$\frac{d^2u}{dx^2} = \sum_{n=0}^N a_n^{(2)} T_n(x) \quad (4.89)$$

After substitution, the Chebyshev inner product is taken.

$$a_n^{(2)} + \lambda^2 a_n = 0 \quad \text{for } 0 \leq n \leq N-2 \quad (4.90)$$

$$\sum_{n=1}^N (n^2 a_n + h a_n) = 0 \quad (4.91)$$

$$\sum_{n=1}^N (-1)^n a_n = 0 \quad (4.92)$$

Equations (4.90) - (4.92) can now be written in matrix form.

$$\begin{pmatrix} \mathbf{E}^2 \\ n^2 I \\ (-1)^n I \end{pmatrix} \mathbf{a} = h \begin{pmatrix} \mathbf{0} \\ -I \\ 0 \end{pmatrix} \mathbf{a} \quad (4.93)$$

The generalized eigenvalue problem was solved using MathCad[®]. Table 4.2 gives the eigenvalue h for different values of N .

Table 4.2 The eigenvalue h for Example 4.4 for various values of N .

N	5	6	7	8	9	10	15	Actual
λ	8.115	-1.885	-0.3182	0.4461	0.5772	0.5853	0.5883	0.5883

Note that in this example, there was only one eigenvalue to be found. In general, the number of eigenvalues that will be found will be equal to the rank of the left hand matrix or the right hand matrix, whichever is smaller. Here the rank of the right hand matrix is equal to 1, which is the number of eigenvalues found.

The next and last example will demonstrate an actual application of this method to the Nield problem [7]. The Nield problem is the solution of the onset of fluid convection in a single layer of liquid. The liquid layer is either heated from above or below by a heating plate. The upper surface of the liquid is free to deflect and is exposed to air (or some other gas).

Example 4.5. *Given the following system, solve for the critical Marangoni number (Ma) which corresponds with the onset of fluid convection.*

$$(D^2 - \omega^2)^2 W = \omega^2 Ra \Theta \quad (4.94)$$

$$(D^2 - \omega^2) \Theta = -W \quad (4.95)$$

The system needs six boundary conditions plus an additional equation for the deflection of the gas-liquid interface, ς .

$$W(-1) = 0 \quad (4.96)$$

$$DW(-1) = 0 \quad (4.97)$$

$$\Theta(-1) = 0 \quad (4.98)$$

$$W(0) = 0 \quad (4.99)$$

$$(D^2 - 3\omega^2) DW(0) - \left[Ra + \frac{G + \omega^2}{C} \right] \omega^2 \varsigma = 0 \quad (4.100)$$

$$D^2W(0) - \omega^2 Ma [\varsigma(0) - \Theta(0)] = 0 \quad (4.101)$$

$$D\Theta(0) + L[\Theta(0) - \varsigma] = 0 \quad (4.102)$$

The system of equations has been non-dimensionalized and linearized using a linear stability analysis. The time derivative has been eliminated using a Fourier expansion. Because we are only interested in the steady solutions, the time constant is set equal to zero. The problem will be set up so that the Marangoni Number, Ma , is the eigenvalue. Here D is the derivative $\frac{d}{dz}$, W is the velocity, Θ is the temperature, ω is the wave number corresponding to the perturbation, Ra is the Rayleigh number, G is the Weber number, C is the Crispation number, Ma is the Marangoni number, L is the Biot number and ς is the surface deflection term. For a complete derivation, the interested reader is referred to the paper by Nield. In Nield's paper, the surface deflection is neglected. Here the surface is allowed to deflect. Values for the deflecting case have been calculated [10].

Again we need to stretch the coordinates from $0 \leq z \leq 1$ to $-1 \leq x \leq 1$, using the stretching function, $x = 2z + 1$. Apply the Chebyshev polynomial interpolation.

$$W = \sum_{n=0}^N a_n T_n(x) \quad (4.103)$$

$$\Theta = \sum_{m=0}^M b_m T_m(x) \quad (4.104)$$

After substitution, the inner product is taken.

$$(16\mathbf{E}^4 - 8\omega^2\mathbf{E}^2 + \omega^4\mathbf{I}) \cdot \mathbf{a} - \omega^2 Ra \mathbf{I} \cdot \mathbf{b} = 0 \quad (4.105)$$

$$(4\mathbf{E}^2 - \omega^2\mathbf{I}) \mathbf{b} + \mathbf{a} \cdot \mathbf{I} = 0 \quad (4.106)$$

$$\sum_{n=0}^N (-1) a_n = 0 \quad (4.107)$$

$$\sum_{n=1}^N (-1)^{n+1} n^2 a_n = 0 \quad (4.108)$$

$$\sum_{m=0}^M (-1) b_m = 0 \quad (4.109)$$

$$\sum_{n=0}^N a_n = 0 \quad (4.110)$$

$$8 \sum_{n=3}^N \left[\frac{n^2}{27} (n^2 - 1) (n^2 - 4) \right] - 6\omega^2 \sum_{n=1}^N n^2 a_n - \left[Ra + \frac{G + \omega^2}{C} \right] \omega^2 \zeta = 0 \quad (4.111)$$

$$4 \sum_{n=2}^N \frac{n^2}{3} (n^2 - 1) a_n - \omega^2 Ma \left(\sum_{m=0}^M \zeta - b_m \right) = 0 \quad (4.112)$$

$$2 \sum_{m=1}^M m^2 b_m + L \sum_{m=0}^M b_m - L\zeta = 0 \quad (4.113)$$

\mathbf{E}^4 can be found by using equation (3.49). The strange products in (4.111) and (4.112) are the result of the third and second order derivative in equation (3.35).

There are several interesting points to be made at this time. In (4.105), the inner product of the equation restricts the number of terms that $\mathbf{b} = \{b_m : m = 0, 1, \dots, M\}$ could have, which is the number of inner products taken. Here we will choose $N - 4$. The number $N - 4$ corresponds to the choice of N and that there are 4 boundary conditions associated with (4.105). The same situation holds for (4.106). Again we will choose N but here there are only two boundary conditions associated with the equation, which gives $N - 2$ equations. Equation (4.105) applies restrictions to the choice of M . When the inner product of the equation is taken, Θ_N must lie in W_N and vice versa.

For simplification and in general, we will let $N = M$ and truncate the indices accordingly. With this in mind, equations (4.105) through (4.112) can be rewritten.

$$(16\mathbf{E}^4 - 8\omega^2\mathbf{E}^2 + \omega^4\mathbf{I}) \cdot \mathbf{a} - \omega^2 Ra\mathbf{I} \cdot \mathbf{b} = 0 \quad (4.114)$$

$$(4\mathbf{E}^2 - \omega^2\mathbf{I}) \mathbf{b} + \mathbf{a} \cdot \mathbf{I} = 0 \quad (4.115)$$

$$\sum_{n=0}^N (-1) a_n = 0 \quad (4.116)$$

$$\sum_{n=1}^N (-1)^{n+1} n^2 a_n = 0 \quad (4.117)$$

$$\sum_{m=0}^N (-1) b_m = 0 \quad (4.118)$$

$$\sum_{n=0}^N a_n = 0 \quad (4.119)$$

$$8 \sum_{n=3}^N \left[\frac{n^2}{27} (n^4 - 5n^2 + 4) \right] - 6\omega^2 \sum_{n=1}^N n^2 a_n - \left[Ra + \frac{G + \omega^2}{C} \right] \omega^2 \varsigma = 0 \quad (4.120)$$

$$4 \sum_{n=2}^N \frac{n^2}{3} (n^2 - 1) a_n - \omega^2 Ma \left(\sum_{m=0}^N \varsigma - b_m \right) = 0 \quad (4.121)$$

Now write (4.113) through (4.120) in matrix form.

$$\begin{pmatrix} 16\mathbf{E}^4 - 8\omega^2\mathbf{E}^2 + \omega^4\mathbf{I} & -\omega^2 Ra\mathbf{I} & 0 \\ \mathbf{I} & 4\mathbf{E}^2 - \omega^2\mathbf{I} & 0 \\ (-1)^n I & 0 & 0 \\ (-1)^n n^2 I & 0 & 0 \\ 0 & (-1)^n & 0 \\ I & 0 & 0 \\ 8\frac{n^2}{27} (n^4 - 5n^2 + 4) - 6\omega^2 n^2 & 0 & -\left(Ra + \frac{G + \omega^2}{C} \right) \omega^2 \\ \frac{4n^2}{3} (n^2 - 1) & 0 & 0 \\ 0 & (2n^2 + L) I & -L \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \\ b_0 \\ \vdots \\ b_n \\ \varsigma \end{pmatrix} = Ma \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & -\omega^2 I & \omega^2 \\ 0 & 0 & 0 \end{pmatrix} \begin{pmatrix} a_0 \\ a_1 \\ \vdots \\ a_n \\ b_0 \\ \vdots \\ b_n \\ \varsigma \end{pmatrix} \quad (4.122)$$

The first row of both matrices in (4.122) has actually $N - 3$ entries and the second row has $N - 1$ entries. The first and second column has N entries, and the last column has only one entry. The FORTRAN program used to set up and solve for the above generalized eigenvalue problem is given in the appendix. One of the subroutines was called from an IMSL subroutine library.

5. Summary

I hope that this paper has helped to demonstrate the usefulness of Chebyshev Spectral Tau methods. Of course there is no such thing as a free lunch. It becomes obvious that the implementation of this method is more complicated than a finite difference method. The Chebyshev Spectral Tau method is most useful for problems which may need to be solved for many times or when a parameter in the problem needs to be changed often. The usefulness of spectral methods was also demonstrated for eigenvalue problems.

In section two, the Chebyshev polynomial properties and the methods of summation were given as background material for the third section. Section three developed the recurrence relationships between functions expanded into Chebyshev polynomials and the derivatives of those expansions. The relationships between the derivatives of the expansion coefficients were used in section four in the spectral tau technique. These recurrence relationships can be found in the appendix of Gottlieb and Orszag's book [5] for various linear operators. If the relationship you are interested in is not tabulated, the techniques given in this paper can be used to generate them. The appendix gives a copy of the FORTRAN program used to solve for the eigenvalues of Nield's problem in Example 4.5. Some of the newer higher level software could also be used to solve these equations. Good examples of these programs are MathCad[®], Maple[®] and Matlab[®].

The intent of this report is to help the beginner or uninitiated start using Chebyshev spectral methods. There are several aspects which were not dealt with. Some of these are singularities in the governing equations, efficient solver methods, such as fast Fourier transforms, and stability. These topics are covered in *Spectral Methods in Fluid Dynamics* [2]. It appears that fourth order and higher differential equations will become unstable. This problem can be worked around by splitting fourth order equations into two second order equations. Even though the fourth order equations are unstable, most problems can still be solved using the Chebyshev Spectral Tau technique. A good example is given in *Numerical Analysis of Spectral Methods* [5] on page 144-145. Some higher order problems,

however do exhibit unstable behavior. I have discovered a system which gives incorrect eigenvalues for only certain values of the system parameters. This system was similar to the Nield problem but dealt with two liquid layers with deflecting surfaces. Whenever possible, it is advised to deal with second order equations only.

[3]

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6. Appendix

PROGRAM NIELD

```

INTEGER I, J, N, M, BC, II
REAL PI, OMEGA, OMEG2, OMEG4
PARAMETER (N = 20, M = 2*N+1, PI = 3.141592654)
REAL B2(N, N), B4(N, N), A(M,M), B(M,M), BETA(N)
REAL VEC0(N), VEC1(N), VEC1N(N), VEC2(N), VEC3(N)
REAL L, MA, RA, OMEGA
REAL TN1, TN2, TN3, TN4, TN0
COMPLEX ALPHA(M), EVEC(M)
* Define the matrices used in defining the large matrices *****
*** INTMAT initializes the matrix entries to zero. *****
CALL INTMAT(B2, 1, N, 1, N)
CALL INTMAT(B4, 1, N, 1, N)
CALL INTMAT(A, 1, M, 1, M)
CALL INTMAT(B, 1, M, 1, M)
***CHDERx gives the  $E^x$  matrix *****
CALL CHDER2(B2, N, N)
CALL CHDER4(B4, N, N)
***CHDERB gives the boundary condition vector *****
CALL CHDERB(VEC0, 0, N, -1)
CALL CHDERB(VEC1, 1, N, 1)
CALL CHDERB(VEC1N, 1, N, -1)
CALL CHDERB(VEC2, 2, N, 1)
CALL CHDERB(VEC3, 3, N, 1)
*Define the parameters to be used. OMEG2, OMEG4, TN1 through *

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*TNP1 are used for optimization puposes *****
OMEGA = 2.13
L = 1.04
G = 0.452
C = 50.9E-5
OMEG2 = OMEGA * OMEGA
OMEG4 = OMEG2 * OMEG2
TN1 = 2 * N - 1
TN2 = 2 * N - 2
TN3 = 2 * N - 3
TN4 = 2 * N - 4
TN0 = 2 * N
** Row 1 Column 1 *****
DO 20 I = 1, N-4
  DO 10 J = I+1, N
    A(I,J) = 16.0 * B4(I,J) - 8.0 * OMEG2 * B2(I,J)
  10 CONTINUE
  A(I,I) = OMEG4
20 CONTINUE
** Row 1 Column 2 *****
DO 30 I = 1, N-4
  A(I, I+N) = -OMEG2 * RA
30 CONTINUE
** Row 2 Column 1 *****
DO 40 I = 1, N-2
  A(I+N-4,I) = 1.0
40 CONTINUE
** Row 2 Column 2 *****
DO 60 I = 1, N-2
  II = I+N-4
  DO 50 J = I+1, N
    A(II,J+N) = 4.0 * B2(I,J)
  50 CONTINUE
  A(II, I+N) = -OMEG2
60 CONTINUE
** Boundary Conditions *****
DO 100 J = 1, N

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A(TN4,J) = VEC0N(J)
A(TN3,J) = VEC1N(J)
A(TN2,J+N) = VEC0N(J)
A(TN1,J) = 8.0 * VEC3(J) - 6.0 * OMEG2 * VEC1(J)
A(TN0,J) = 4.0 * VEC2(J)
A(M,J+N) = L
A(M,J) = 2.0 * VEC1(J)
100 CONTINUE
A(TN1,M) = -OMEG2 * (RA + (G + OMEG2) / C)
A(M,M) = -1.0
*****
*** Now assign values to the B matrix *****
DO 200 J = 1, N
  B(TN0,J+N) = -OMEG2
200 CONTINUE
B(TN0,M) = OMEG2
*****
*The subroutine GVLRG is linked and called from ISML library.
*M is the size of the matrix, ALPHA is a vector of numerators of the
*eigenvalues, and BETA is a vector of denominators of the eigenvalues.
*****
CALL GVLRG(M, A, M, B, M, ALPHA, BETA)
DO 200 J = 1, M
  IF (BETA(J) .EQ. 0) THEN
    EVEC(J) = 12345
  ELSE
    EVEC(J) = ALPHA(J) / BETA(J)
  END IF
200 CONTINUE
END
*****
* This subroutine evaluates the derivatives of a Chebyshev polynomial
* at a boundary point of 1 or -1. It returns the vector of
* coefficients that are associated with it in VECTOR.
* VECTOR is the vector returned
* ORDER is the order of the derivative
* LENGTH is the length of the vector VECTOR

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* EVAL is the point at which the derivative is evaluated
SUBROUTINE CHDERB (VECTOR, ORDER, LENGTH, EVAL)
INTEGER ORDER, LENGTH, K, N, EVAL, N2
REAL VECTOR(LENGTH), PROD
IF (EVAL .EQ. -1) THEN
DO 20 N = 0, LENGTH-1
  PROD = 1.0
  N2 = N * N
  DO 10 K = 0, ORDER - 1
    PROD = PROD * (N2 - K*K) / (2.0 * K + 1)
  10 CONTINUE
  VECTOR(N+1) = (-1.0)**(N+ORDER) * PROD
20 CONTINUE
ELSE IF (EVAL .EQ. 1) THEN
DO 40 N = 0, LENGTH-1
  PROD = 1.0
  N2 = N * N
  DO 30 K = 0, ORDER - 1
    PROD = PROD * (N2 - K*K) / (2.0 * K + 1)
  30 CONTINUE
  VECTOR(N+1) = PROD
40 CONTINUE
ELSE
PRINT *, 'Boundary condition evaluated at'
PRINT *, 'value other than 1 or -1.'
PAUSE 'Executing in subroutine CHDERB'
END IF
END
*****
* This subroutine finds the coefficient matrix associated with
* the first derivative of the Chebyshev series
* ROWS is the number of rows in the matrix
* COLUMNS is the number of columns in the matrix
* I and J are indices used.
* MATRIX is the matrix that is passed back to the main program
* MATRIX has size (1:ROWS, 1:COLUMNS)
*****

```

```

SUBROUTINE CHDER1 (MATRIX, ROWS, COLUMNS)
INTEGER I, K, ROWS, COLUMNS
REAL MATRIX(ROWS, COLUMNS)
CK = 2
DO 10 I = 1 , ROWS
  DO 20 J = I + 1 , COLUMNS , 2
    MATRIX(I, J) = 2 / CK * (J - 1)
  20 CONTINUE
  CK = 1
10 CONTINUE
END
*****
* This subroutine finds the coefficient matrix associated with
* the second order derivatives of the Chebyshev series
* ROWS is the number of rows in the matrix
* COLUMNS is the number of columns in the matrix
* I and J are indices used.
* MATRIX is the matrix that is passed back to the main program
* MATRIX has size (1:ROWS, 1:COLUMNS)
*****
SUBROUTINE CHDER2 (MATRIX, ROWS, COLUMNS)
INTEGER I, K, ROWS, COLUMNS
REAL MATRIX(ROWS, COLUMNS)
CK = 2
DO 10 I = 1 , ROWS
  DO 20 J = I + 2 , COLUMNS , 2
    MATRIX(I, J) = ((J-1) * ((J-1)**2 - (I-1)**2)) / CK
  20 CONTINUE
  CK = 1
10 CONTINUE
END
*****
* This subroutine finds the coefficient matrix associated with
* the fourth order derivatives of the Chebyshev series
* MATRIX has size (1:ROWS, 1:COLUMNS)
* MATRIX = the matrix to be passed back assigned with the value
* of fourth order coefficients

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* ROWS = the length of the rows of MATRIX
* COLUMNS = the number of the columns of MATRIX
*****
SUBROUTINE CHDER4(MATRIX, ROWS, COLUMNS)
INTEGER I, J, ROWS, COLUMNS
REAL MATRIX(ROWS, COLUMNS), A, B, C, D
CK = 2
DO 20 I = 0, ROWS-1
  D = I**2 * (I**2 - 4)**2
  DO 10 J = I + 4, COLUMNS-1, 2
    A = J**2 * (J**2 - 4)**2
    B = 3.0 * I**2 * J**4
    C = 3.0 * I**4 * J**2
    MATRIX(I+1, J+1) = J*(A - B + C - D) / (CK * 24)
  10 CONTINUE
  CK = 1
20 CONTINUE
END
*****
* This subroutine initializes all the entries of a matrix
* ROWS is the number of rows in the matrix
* COLUMNS is the number of columns in the matrix
* I and J are indices used.
*****
SUBROUTINE INTMAT (MATRIX, ROW1, ROWEND, COL1, COLEND)
INTEGER I, J, ROW1, ROWEND, COL1, COLEND
REAL MATRIX(ROW1:ROWEND, COL1:COLEND)
DO 20 J = COL1 , COLEND
  DO 10 I = ROW1 , ROWEND
    MATRIX(I, J) = 0.0
  10 CONTINUE
20 CONTINUE
END

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