SPURIOUS EIGENVALUES IN THE SPECTRAL TAU METHOD

by

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SPURIOUS EIGENVALUES IN THE SPECTRAL TAU METHOD

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The Chebyshev-tau method is a popular and useful method for approximating solutions to boundary value problems. For certain stability problems the method yields a set of "spurious eigenvalues". In these problems all of the eigenvalues are known to be negative, but the Chebyshev-tau methods returns at least one *positive* eigenvalue along with approximations to the actual eigenvalues. These eigenvalues clearly do not belong and so historically have been called spurious eigenvalues. The spurious eigenvalues can lead to a false assumption that a system is unstable when in reality it is not. In the past spurious eigenvalues were assumed to be due to discretization errors that would disappear for large enough truncation order or they were eliminated *ad-hoc*.

In this work a model problem that is simple enough to easily work with, yet exhibits the desired behavior is studied. Gegenbauer polynomials will be used in the tau method in order to simultaneously study a range of tau methods that include the Chebyshev- and Legendre-tau methods. It will be shown that when the Legendre-tau method is used to approximate the eigenvalues of the model problem an infinite generalized eigenvalue arises for every truncation order. Using generalized

eigenvalue theory it will also be shown that for a range of Gegenbauer polynomials, including the Chebyshev polynomials, the Gegenbauer-tau method produces an approximation to this infinite generalized eigenvalue for every truncation order. This approximation will be shown to grow, in magnitude, like N^4 where N is the truncation order of the method. Hence, it will be shown that the spurious eigenvalues are not numerical errors, but in fact belong in the solution for every truncation order.

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Contents

Chapter 1

Introduction

Spectral tau methods have been successfully used for the last 20 years to numerically solve differential eigenvalue problems. In some instances however the solution given by the tau method includes a set of "spurious eigenvalues" along with approximations to the actual eigenvalues of the problem. In particular, when the Chebyshev-tau method is used to approximate the eigenvalues from several hydrodynamic stability problems it yields approximations to the actual eigenvalues, which are known to be negative, and at least one *positive* eigenvalue that grows as the truncation order grows.

In a stability analysis positive eigenvalues indicate that a disturbance will grow exponentially and hence the solution will be unstable. The presence of these "spurious eigenvalues" then could cause one to erroneously assume that the solution had unstable modes when in reality it does not. The net effect then of spurious eigenvalues is to cast doubt on the accuracy of a very useful approximation method. Explaining the existence of these spurious eigenvalues will then help in the future to identify or eliminate the spurious eigenvalues thus allowing the analysis of a given problem to proceed.

In the past spurious eigenvalues were either eliminated *ad hoc* or assumed to be numerical discretization problems that would disappear if the truncation order was increased enough. The *ad hoc* methods, while eliminating the positive approximations, introduced at least one negative approximation that rapidly increased in magnitude as the truncation order increased. Since this new approximation from the *ad-hoc* methods was not positive it was ignored.

In this work a model problem which displays this behavior and is relatively simple to work with is examined. It will be shown that when applying the Chebyshev-tau method to the model problem spurious eigenvalues will arise for all truncation orders and hence are not a numerical artifact. In fact it will be shown that spurious eigenvalues exist at all truncation orders for a range of spectral-tau methods.

Along with the proof of the existence of the spurious eigenvalues in the model problem an explanation for why the spurious eigenvalues arise will be given. It will be shown that the spurious eigenvalues are an approximation of an "infinite eigenvalue" from a "near-by" generalized eigenvalue problem that arises from the

application of the Legendre-tau method to the model problem. This explanation will give insights into why the *ad-hoc* methods work.

This work will start with a description of the model problem. This will be followed with a discussion of the spectral tau method applied to the model problem. In particular, the tau method using Gegenbauer (ultraspherical) polynomials will be discussed. The Gegenbauer polynomials are a family of orthogonal polynomials that include both the Chebyshev and Legendre polynomials as special cases. Hence, using the Gegenbauer-tau method will include both the Chebyshev- and Legendre-tau methods.

Following this the existence of the spurious eigenvalues is proved for a range of Gegenbauer-tau methods. This will be done using two different methods. The first method is a functional analytic method and will allow the existence of the spurious eigenvalues to be proven for a range of Gegenbauer-tau methods. This method however does not give an adequate explanation for their existence.

The second method will make use of generalized eigenvalue theory to prove the existence of spurious eigenvalues in the model problem. More importantly however, the method will provide an explanation for the existence of the spurious eigenvalues. This method will show the Legendre-tau method yields an infinite generalized eigenvalue for every truncation order. Furthermore, it will be shown that for a range of Gegenbauer polynomials, including the Chebyshev polynomials, the tau method will yield approximations to this infinite generalized eigenvalue. These will then be the spurious eigenvalues.

Chapter 2

The Gegenbauer-tau Approximation Method

2.1 Model Problem

The work in this dissertation concerns the application of the spectral-tau method to the model eigenvalue problem

$$u^{(4)} = su'' \qquad -1 < x < 1 \tag{2.1}$$

$$u(-1) = u(1) = u'(-1) = u'(1) = 0.$$

This model problem provides an example that is easy to analyze in which spurious eigenvalues occur when the Chebyshev-tau method is applied. The model problem arises from a separation of variables applied to a one-dimensional model of the vorticity-streamfunction equations for low Reynolds number incompressible flow [1, pages 143-144]. This particular problem has also been studied in the past in [2, 3, 4, 5].

The eigenvalues of this model problem are all negative and satisfy $s = -n^2\pi^2$ or $\tan\left(\sqrt{-s}\right) = \sqrt{-s}$. The first five eigenvalues are

$$\begin{aligned} s_1 &= -\pi^2 \approx -9.869604401 \\ s_2 &\approx -20.19072856 \\ s_3 &= -4\pi^2 \approx -39.47841760 \\ s_4 &\approx -59.67951594 \\ s_5 &= -9\pi^2 \approx -88.8264396098. \end{aligned}$$

The corresponding eigenfunctions are

$$1 + (-1)^{n+1}\cos(n\pi x)$$

and

$$-\sqrt{-s}\cos(\sqrt{-s}\,x) + \sin\left(\sqrt{-s}\,x\right)$$

respectively. Application of the Chebyshev-tau method to this model problem produces two large positive eigenvalues that grow as the order of approximation grows. Table 2.1 shows the results of the first six orders of approximation using the Chebyshev-tau method. It can be seen that two positive eigenvalues are computed

N	1	2	3	4	5	6
N^4	1	16	81	256	625	1296
	40.	251.453	529.388	1331.132	2284.474	4272.17
	12.	40.	251.453	529.388	1331.132	2284.47
		−11.453	−11.453	−9.892	−9.892	−9.870
eigenvalues			−25.388	−25.388	−20.338	−20.338
				−61.239	−61.239	−40.663
					−104.136	−104.136
						−189.638

Table 2.1: Eigenvalues for the model problem, (2.1), computed using the Chebyshev-tau method

and that they grow faster than N^4 where N is the order of approximation in the Chebyshev-tau method. The negative eigenvalues appear to be converging to the correct values for the model problem, (2.1). Notice also that the eigenvalues "leap-frog" as the order of approximation increases. The largest eigenvalue in column N becomes the second largest eigenvalue in column $N+1$ and the smallest negative eigenvalue in column N becomes the next to last eigenvalue in column $N+1$. This behavior is due to the parity structure of the problem (see Section 2.3). For an expanded table of eigenvalues for higher orders of approximation see [1, 3].

Historically spurious eigenvalues were defined to be positive eigenvalues that arises in an approximation to a problem where it is known that no positive eigenvalues exist. For this work a different definition will be used.

Definition 2.1.1 *A spurious eigenvalue is a large magnitude eigenvalue that grows rapidly as the truncation order increases.*

This new definition is preliminary and will be made more specific in Section 5.5 after a detailed analysis of the problem has been performed. Note that this definition of the spurious eigenvalue includes both positive and negative eigenvalues. The reason for including negative eigenvalues in this definition will be made clear in Section 5.5.

An understanding of this problem could help with the understanding of several other problems that are similar to the model problem (2.1) in structure. One such problem is

$$D^2u = sDu \qquad r_1 < r < r_2$$
$$u(r_1) = u(r_2) = u'(r_1) = u'(r_2) = 0$$

where the second-order differential operator, D, is

$$Du = u'' + \frac{2}{r}u' - \frac{l(l+1)u}{r^2}.$$

This boundary value problem arises from a hydrodynamic stability analysis in spherical coordinates. When the Chebyshev-tau method is applied to this problem spurious eigenvalues also arise, see [2, 6, 7]. Another example of a structurally similar problem is the Orr-Sommerfeld stability equation for plane Poiseuille flow

$$\frac{u^{(4)} - 2\alpha^2 u'' + \alpha^4 u}{-i\alpha R} + \left[(U - s)(u'' - \alpha^2 u) - U'' u\right] = 0 \qquad -1 < x < 1$$

$$u(-1) = u(1) = u'(-1) = u'(1) = 0$$

where u is the amplitude of the velocity disturbance, α is the wave number, R is the Reynolds number, and $U(x) = 1 - x^2$ is the known steady base flow. For this problem the stability of the base flow is being examined and the stability parameter is the Reynolds number, R. It is important in this problem to know the value of R where at least one eigenvalue has a positive real part. See [2, 8, 5] for the details of this problem. When the Chebyshev-tau method is applied to this problem two spurious eigenvalue with large imaginary parts are produced (see [2] for details).

The Orr-Sommerfeld stability problem is structurally similar to the model problem (2.1) in that

$$\frac{u^{(4)} - 2\alpha^2 u'' + \alpha^4 u}{-i\alpha R}$$

is a fourth order differential operator and

$$\left[(U - s)(u'' - \alpha^2 u) - U'' u\right]$$

is a second order differential operator. The boundary conditions are also similar.

2.2 The tau Method

The tau method uses a truncated series expansion in a complete set of orthogonal functions as an approximation to the solution of an ordinary differential equation. The tau method was first proposed as a way of solving boundary value problems without requiring the basis functions to satisfy the boundary conditions by Lanczos in [9, 10]. The use of Chebyshev polynomials in the tau method was extensively developed by Fox in [11, 12]. The tau method was extended by Ortiz in [13] for the use of canonical polynomials. Boyd [14, Chapter 18] has a more detailed history of the tau method.

To illustrate the tau method, first consider the boundary value problem

$$L\{u\} = 0 \qquad -1 < x < 1 \tag{2.2}$$

$$B_i\{u(-1)\} = B_j\{u(1)\} = 0 \qquad i + j = N_b \tag{2.3}$$

where L is a linear ordinary differential operator, $u(x)$ is an unknown function, and B_i and B_j are linear operators which represent the boundary conditions. The subscript i on B_i denotes the number of boundary conditions applied at $x = -1$.

Similarly, the subscript j denotes the number of boundary conditions applied at $x = 1$.

Let $u(x)$ be approximated as follows:

$$u(x) \approx u(x, M) = \sum_{k=0}^{M+N_b} a_k f_k(x) \tag{2.4}$$

where the a_k's are unknown coefficients and the f_k's are functions from the complete orthogonal set with inner product $\langle \cdot, \cdot \rangle$. Substitute (2.4) into (2.2) and use linearity to interchange the summations with the operator, L. Now, taking the inner product of this new equation with f_l for $l = 0, 1, \ldots, M$ gives a system of $M + 1$ equations in the unknowns a_k, $k = 0, 1, \ldots, M + N_b$. In order to actually find the a_k's then, N_b more equations are needed. These remaining equations come from the substitution of (2.4) into the boundary conditions (2.3). This results in a system of $M + N_b + 1$ equations which are linear in the a_k's. The system that is produced is

$$\sum_{k=0}^{M+N_b} a_k \langle L\{f_k(x)\}, f_l\rangle = 0 \qquad l = 0, 1, \ldots, M \tag{2.5}$$

$$\sum_{k=0}^{M+N_b} a_k B_i\{f_k(-1)\} = \sum_{k=0}^{M+N_b} a_k B_j\{f_k(1)\} = 0 \qquad i + j = N_b. \tag{2.6}$$

If the problem is an eigenvalue problem, then the unknown eigenvalue will appear in the matrix equation corresponding to (2.5) and (2.6). Standard matrix and eigenvalue solvers can then be used to solve (2.5) and (2.6).

Notice that the tau method is really solving a nearby, or approximate, differential equation exactly with a polynomial. The tau method applied to a constant coefficient linear differential equation will exactly solve the following residual problem, namely

$$L\{u\} = \sum_{k=1}^{N_b} \tau_k f_{M+k}(x) \tag{2.7}$$

$$\sum_{k=0}^{M+N_b} a_k B_i\{f_k(-1)\} = \sum_{k=0}^{M+N_b} a_k B_j\{f_k(1)\} = 0 \qquad i + j = N_b. \tag{2.8}$$

where the coefficients τ_k for $k = 1, \ldots, N_b$ are called the tau coefficients and are unknown. These coefficients also account for the name of the method. The residual of the problem

$$\sum_{k=1}^{N_b} \tau_k f_{M+k}(x),$$

is a measure of the ability of $u(x, M)$ to satisfy the original differential equation.

Substituting the approximation, $u(x, M)$, into (2.7) and then taking the inner product against the functions f_k for $k = 0, 1, \ldots, M + N_b$ gives the following system

of equations

$$\left\langle L\{u(x,M)\}, f_k\right\rangle = 0 \qquad k = 0,1,\ldots,M \tag{2.9}$$

$$\left\langle L\{u(x,M)\}, f_{M+k}\right\rangle = \tau_k \left\langle f_{M+k}, f_{M+k}\right\rangle \qquad k = 1,\ldots,N_b. \tag{2.10}$$

Then after solving (2.5) and (2.6) for the a_k's, (2.10) can be used to find the tau coefficients. It has been shown by Fox [11] that the tau coefficients give error bounds on the approximate solution $u(x,M)$. Since the Chebyshev polynomials are bounded in absolute value by 1 on the interval $[-1,1]$ the error introduced by the Chebyshev-tau method will be small if the tau coefficients are small. The tau coefficients are rarely calculated in practice, although they have been used to identify spurious eigenvalues (see [2] for details).

2.3 The tau Method Applied to the Model Problem

Orszag, in [8], applied and advocated the Chebyshev-tau method for a wide variety of problems. Chebyshev polynomials are very well suited for use in the tau method. The Chebyshev polynomials are orthogonal and form a complete set. Also, the Chebyshev polynomials have a nearly optimal uniform approximation of continuous functions [15]. The work in this dissertation however, takes a slightly more general approach. Instead of using Chebyshev polynomials exclusively in the tau method we will use Gegenbauer, or ultraspherical, polynomials. The advantage of using Gegenbauer polynomials is that many of the common orthogonal polynomial sets, including Chebyshev polynomials, are special cases of the Gegenbauer polynomials. Also, the use of Gegenbauer polynomials will allow results to be found for whole ranges of orthogonal polynomial sets instead of just the Chebyshev polynomials. This is not to imply that Gegenbauer polynomials should be used in the tau method for numerical calculations, but many of the theoretical results later in this dissertation will need a general Gegenbauer polynomial setting instead of a Chebyshev polynomial setting. In fact, the main theorem in Section 5.5 proving the existence of a spurious eigenvalue for the application of the Chebyshev-tau method is only made possible due to the more general setting.

Before the actual application of the Gegenbauer-tau method to the model problem, (2.1), a brief digression into Gegenbauer polynomials is needed. The Gegenbauer polynomials are a general family of polynomials which are defined in the following way. Let $x \in [-1,1]$, $\nu \in (-\frac{1}{2},\infty)$ and n be a natural number, then

$$G_n^\nu(x) = (-1)^n \sum_{j=0}^{\lfloor n/2 \rfloor} \binom{-\nu}{n-j}\binom{n-j}{j}(2x)^{n-2j}.$$

As mentioned above, some common sets of orthogonal polynomials are special cases

of the Gegenbauer polynomials. For example:

$T_n(x) = \frac{n}{2} \lim_{\nu\to 0} \frac{G_n^\nu(x)}{\nu}$	Chebyshev polynomials of the first kind
$U_n(x) = G_n^1(x)$	Chebyshev polynomials of the second kind
$P_n(x) = G_n^{\frac{1}{2}}(x)$	Legendre polynomials

The presence of the limit in the representation of the Chebyshev polynomials of the first kind in terms of Gegenbauer polynomials presents some difficulties with most of the calculations that are to follow. Many of the calculations to follow will involve terms containing $\Gamma(\nu)$ or $\Gamma(2\nu)$ and so it is impossible to take the limit by simply substituting $\nu = 0$ into the equations. The limit and the presence of the $1/\nu$ in the limit is required in order to handle the $\Gamma(\nu)$ that is present in many of the formulas. Therefore, due to the importance and widespread use of the Chebyshev-tau method, the case of the Chebyshev polynomials of the first kind will be examined separately after the general case has been considered.

Now, given the weight function

$$w(x) = (1 - x^2)^{\nu - \frac{1}{2}},$$

and defining the inner product to be the usual weighted inner product

$$\langle f(x), g(x)\rangle = h_n \int_{-1}^{1} f(x)\, g(x)\, w(x)\, dx$$

the Gegenbauer polynomials are an orthonormal set of polynomials [16, pages 773 and 774]. Here

$$h_n = \begin{cases} \dfrac{n!\,(n+\nu)\ [\Gamma(\nu)]^2}{\pi\, 2^{1-2\nu}\, \Gamma(n+2\nu)} & \nu \neq 0 \\[2ex] \dfrac{2}{\pi} & \nu = 0 \end{cases}$$

Note that Abramowitz and Stegun [16] actually give

$$h_n = \frac{n^2}{2\pi}$$

as the normalizing factor for $\nu = 0$ but they do not use the $\frac{n}{2}$ in the definition of the Chebyshev polynomials.

Also the Gegenbauer polynomials are eigenfunctions of the ultraspherical differential equation [17, page 247]

$$\frac{d}{dz}\left[(1 - z^2)^{\nu+1} \frac{du}{dz}\right] + n(n + 2\nu + 1)(1 - z^2)^{\nu} u = 0,$$

which is a regular Sturm-Liouville equation on $-1 < z < 1$ and so the Gegenbauer polynomials are complete [17, page 313]. Therefore the Gegenbauer polynomials can indeed be used in the tau method.

Some terminology concerning the case of Chebyshev polynomials needs to be introduced before proceeding. The case of the Chebyshev polynomials of the first kind will often be referred to in this dissertation as the $\nu = 0$ case or the Chebyshev polynomial case. It must be remembered that whenever either of these statemtents are made they always imply the limiting process that is involved in the Gegenbauer representation of the Chebyshev polynomials of the first kind.

Before proceeding with the actual application of the Gegenbauer-tau method to the model problem a few of reductions allowed by the model problem are made.

The boundary conditions of the model problem allow the first reduction. In the tau method, applied to this problem, a polynomial of degree $M + 4$ is sought that approximately solves the model problem in the sense that it is orthogonal to the basis functions $G_0^\nu(x), G_1^\nu(x), \ldots, G_M^\nu(x)$. This polynomial must also satisfy the boundary conditions. The boundary conditions imply that the approximate solution must have a root of multiplicity 2 at $x = -1$ and a root of multiplicity two at $x = 1$. Hence, it must be possible to factor out $(1 - x)^2(1 + x)^2 = (1 - x^2)^2$ from the approximate solution. Therefore, the final solution will have the form

$$\begin{aligned} u(x, M) &= (1 - x^2)^2 \left(d_0 G_0^\nu(x) + \cdots + d_M G_M^\nu(x)\right) \\ &= d_0(1 - x^2)^2 G_0^\nu(x) + \cdots + d_M(1 - x^2)^2 G_M^\nu(x) \end{aligned}$$

for some constants $d_0, \ldots, d_M$. This means that we can solve for the approximation in terms of the basis functions

$$(1 - x^2)^2 G_k^\nu(x).$$

This also means that (2.6) will be trivially satisfied by the approximation and so we only need to solve (2.5). With this reduction the model problem (2.1) is recast into a Galerkin-Gegenbauer-tau method.

Next, notice that the derivatives in the differential equation in the model problem, (2.1), are of even order. Hence, any even polynomial inserted into the differential equation will remain even, and similarly for odd polynomials. Now, Gegenbauer polynomials of even index are even polynomials and Gegenbauer polynomials of odd index are odd polynomials. Multiplying a Gegenbauer polynomial by $(1 - x^2)^2$ will not change this. Therefore, when using basis functions of the form $(1 - x^2)^2 G_k^\nu(x)$ the parity of the individual terms will not change. This has the effect of partitioning the problem given by (2.5) into a portion involving only even polynomials and a portion involving only odd polynomials. These portions will be referred to as the even and odd portions. So, for truncation order of $M = 2N$ the approximation will now take the form

$$u(x, M) = \sum_{k=0}^{N} d_k(1 - x^2)^2 G_{2k}^\nu(x) + \sum_{k=0}^{N-1} b_k(1 - x^2)^2 G_{2k+1}^\nu(x), \tag{2.11}$$

and for a truncation order of $M = 2N + 1$ the approximation will take the form

$$u(x, M) = \sum_{k=0}^{N} d_k(1 - x^2)^2 G_{2k}^\nu(x) + \sum_{k=0}^{N} b_k(1 - x^2)^2 G_{2k+1}^\nu(x). \tag{2.12}$$

In both of these approximations the first summation is the even portion and the second summation is the odd portion. Partitioning the problem in this manner allows each portion to be examined separately. For simplicity, only the even portion of the model problem is examined here. The odd portion will yield similar results.

Now suppose that we start with a truncation order of $M = 2N$ and then increase the truncation order by one to $M = 2N + 1$. From (2.11) and (2.12) we see that the even portion will remain the same while the odd portion will increase in size by one from N to $N + 1$. The net effect of this is that the approximations of the eigenvalues received from the even portion will not change since this portion remains the same. The only approximations of the eigenvalues that will change are those arising from the odd portion of the problem. It is this behavior that accounts for the "leap-frogging" of the eigenvalues that was seen in Table 2.1.

Due to the fact that the even portion does not change for truncation orders of $M = 2N$ and $M = 2N + 1$ we will always assume from now on that the truncation order is either $M = 2N$ or $M = 2N + 1$.

We can now proceed with the actual application of the modified Gegenbauer-tau method to the model problem, (2.1). Since we will only be examining the even portion of the problem, the approximation is

$$u(x, N) = \sum_{k=0}^{N} d_k (1 - x^2)^2 G^{\nu}_{2k}(x). \tag{2.13}$$

Note the change in notation. We are now using $u(x, N)$ instead of $u(x, M)$ to represent the approximation since we are only looking at the even portion and we are assuming that the truncation order is either $M = 2N$ or $M = 2N + 1$. As was noted above, (2.6) is trivially satisfied by this approximation and so we only need to solve (2.5). In terms of our new approximation, given by (2.13), Equation (2.5) becomes

$$\sum_{k=0}^{N} d_k \Big\langle L\{(1 - x^2)^2 G^{\nu}_{2k}(x)\}, G^{\nu}_{2l}(x) \Big\rangle = 0 \qquad l = 0, 1, \ldots, N.$$

Again, note that the limit on the summation and on l is now N instead of M. For the model problem, (2.1), the differential operator, L, is

$$L = D^{(4)} - sD^{(2)}$$

where D is the normal ordinary differential operator. Substituting this and simplifying gives the following set of $N + 1$ equations

$$\sum_{k=0}^{N} d_k \left\langle \frac{d^4}{dx^4} \left\{ (1 - x^2)^2 \; G^{\nu}_{2k}(x) \right\}, G^{\nu}_{2i}(x) \right\rangle =$$

$$s \sum_{k=0}^{N} d_k \left\langle \frac{d^2}{dx^2} \left\{ (1 - x^2)^2 \; G^{\nu}_{2k}(x) \right\}, G^{\nu}_{2i}(x) \right\rangle . \tag{2.14}$$