Pseudospectral Methods and Composite Complex Maps for Near-Boundary Critical Points

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The rate of convergence of the pseudospectral approximation to singular linear differential eigenproblems is asymptotically geometric, but is often seriously weakened by the presence of singularities, called critical points or critical latitudes. One remedy is to implement an independent variable transformation which distorts the computational domain into the complex plane and away from the critical point. These complex maps can then be chosen to minimize the effect of the critical points. However, the degree of improvement is limited for critical points near a boundary point, since each contour produced by the complex maps must terminate there to enforce the boundary conditions. In this paper, new complex maps are developed for problems containing a single near-boundary critical point. These new composite complex maps are polynomials of degree 2^p, where $p \geq 1$ is the level of composition. Formulae for the optimal map parameters are deduced analytically and indicate that significant acceleration of the geometric rate of convergence is possible. A test problem is solved to illustrate the technique. Although successful, it is shown that previously ignored algebraic factors in the formula for the error may become significant when utilizing composite complex maps. © 1996 Academic Press, Inc.

1. INTRODUCTION

In a recent paper by Gill and Sneddon [1] the role of complex maps in using pseudospectral methods to solve singular differential eigenproblems was explored. Such equations frequently arise in linear, inviscid, hydrodynamic stability calculations among others [2]. Singularities (often called critical points or critical latitudes) occur when the coefficient of the highest derivative vanishes. If this coefficient is not a one-to-one function of the independent variable, there may be several distinct singularities and their location may not be confined to the real axis.

The importance of these critical points (to the numerical analyst) is that their location, relative to the computational domain, determines the asymptotic rate of convergence of the numerical scheme employed. Roughly speaking, the closer the singularities are, the slower the convergence will be, and for singularities on the computational domain the numerical approximations diverge. This was demonstrated

in Gill *et al.* [3], where both finite difference and pseudospectral methods were used to solve a nondivergent barotropic model of tropical cyclones for various velocity profiles. Both methods became increasingly inaccurate at the upper limit of unstable wavenumbers where the critical points approach the computational domain. This problem does not arise at the lower limit of unstable wavenumbers because as the wave speed approaches zero, the critical point does not approach the real axis (for example, see [1]).

The use of complex maps as a remedy to this problem was initially suggested by Boyd and Christidis [4]. The complex map is an independent variable transformation which distorts the computational domain into one in the complex plane, so that the effect of the singularities on the rate of convergence of the numerical schemes is minimized. Its use was investigated in some detail by Boyd [5] and subsequently by Gill and Sneddon. While it has been demonstrated that the use of complex maps can improve the convergence of pseudospectral methods substantially, the theoretical results also implied that the improvement is limited for critical points located near a boundary point of the computational domain. This is a consequence of the requirement that the complex contour produced by the map must terminate at these boundary points so that the boundary conditions can be enforced in the numerical approximation. This requirement restricts the extent to which the complex contour can avoid the given critical points.

This paper extends the work of [1] by investigating the possibility of taking successive complex maps to improve the accuracy even further. Since the gains from using a single complex map are usually quite substantial, this approach is likely to be of most benefit in the case of near-boundary critical points. The prototype differential equation considered is a second-order, linear, two point boundary value problem on the interval $[-1, 1]$ containing a single critical point near one of the end points. The pseudospectral method is outlined briefly in Section 2, together with the determination of its rate of convergence. The use of complex maps (in particular, the quadratic map) with pseudospectral methods is also described. In Section 3, a new family of maps, called composite maps, is developed

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for problems with near-boundary critical points. A test problem is solved in Section 4 and some conclusions about the effectiveness of these new composite maps are made in Section 5.

2. PSEUDOSPECTRAL METHODS

The prototype eigenproblem considered in [1] was the linear (second-order) ordinary differential equation

$$a_2(y, \lambda)u''(y) + a_1(y, \lambda)u'(y) + a_0(y, \lambda)u(y) = 0, \quad (1)$$

subject to homogeneous Dirichlet boundary conditions

$$u(-1) = u(1) = 0. \quad (2)$$

Here $y \in [-1, 1]$ is the real independent variable and λ and $u(y)$ are the eigenvalue and eigenfunction, respectively. The coefficients $a_i(y, \lambda)$ are known functions of y and can depend linearly on the eigenvalue λ. Extensions for higher order derivatives and Neumann or mixed boundary conditions are straightforward.

In the pseudospectral method the unknown eigenfunction in (1) is approximated by a weighted sum of N trial functions $\{\phi_j(y)\}$, i.e.,

$$u(y) \approx u_N(y) = \sum_{j=1}^{N} a_j \phi_j(y). \quad (3)$$

The expansion coefficients $\{a_j\}$ are determined by requiring that $u_N(y)$ satisfy Eq. (1) at a set of nodes $\{y_i\}$ and that the boundary conditions (2) are satisfied. It is common to choose the trial functions to be orthogonal polynomials such as the Chebyshev polynomials of the first kind. In practice, however, an expansion in Lagrange polynomials based on the nodes $\{y_i\}$ is often simplest. Also, the nodes are usually chosen to be the zeros of an $(N - 2)$th-degree orthogonal polynomial together with $y_1 = -1$ and $y_N = 1$.

Convergence results for the pseudospectral method can be obtained by considering Chebyshev polynomial expansions (Solomonoff and Turkel [6], Boyd [7]). Similar results are available for methods based on Lagrange polynomials (see, for example, Krylov [8]). Errors in the pseudospectral solution of the system (1) and (2) are generated from two sources. First, there is the series truncation error due to the fact that terms for which $j > N$ have been neglected in the expansion (3). Second, there is the discretization error—viz. the difference between the first N terms of the exact solution and the corresponding terms calculated by the pseudospectral solution of (1) and (2). Unfortunately, the discretization error is difficult to compute *a priori*. Empirical evidence supports the notion that the discretization error is roughly of the same order of magnitude as the series truncation error—the so-called "assumption of equal errors" [7]. The calculation of the series truncation error is not straightforward either. However, its asymptotic value depends primarily on the location of the singularities of the solution $u(y)$, which can often be determined by inspection of the differential equation.

For a truncated Chebyshev expansion of the form

$$u(y) \approx u_N(y) = \sum_{j=0}^{N} a_j T_j(y),$$

where $T_j(y) = \cos(j \cos^{-1} y)$, the series truncation error satisfies $E_S(y) = O(|a_N|)$ as $N \to \infty$. Thus the rate of convergence is governed by the behavior of the last retained Chebyshev coefficient. Convergence is said to be geometric, since it can be shown that $a_N = O(N^k \delta^{-N})$, where $\delta \geq 1$ is a constant that depends on the location of the nearest singularity [9]. The algebraic factor, which depends on the nature of this singularity, is often ignored, as the exponential term will dominate for large values of N. The Chebyshev series (and the related pseudospectral method) converges inside the largest ellipse with foci at ± 1 that does not contain any singularities. The constant δ is equal to the sum of the lengths of the semi-major and semi-minor axes of this ellipse, or in terms of the singularities y_c of $u(y)$,

$$\delta = \delta(y_c) = \min_{y_c} \{\max\{|y_c \pm \sqrt{y_c^2 - 1}|\}\}. \quad (4)$$

Complex Maps

The differential equation (1) and eigenfunction $u(y)$ possess a regular singular point, or critical point, at the real or complex point y_c satisfying $a_2(y_c, \lambda) = 0$. The rate of convergence of the pseudospectral solution is determined by the location of this critical point through (4). If it is near the interval $[-1, 1]$, the constant δ decreases significantly and convergence becomes very slow. However, if the computational domain is shifted to a contour in the complex y-plane, away from the critical point, then one could expect the rate of convergence to be improved. This can be achieved by a complex map $y = f(x)$, where $x \in [-1, 1]$ is the new (real) independent variable and f is a complex function. The map $f(x)$ must satisfy $f(\pm 1) = \pm 1$ so that the complex contour will pass through the boundary points at which the boundary conditions are to be enforced. Details of the transformation are given in [1].

The advantage of this approach is that the transformed differential equation (and eigenfunction) will be singular at $x_c = f^{-1}(y_c)$, which, with an appropriate choice of map, may yield a larger value of δ. The disadvantage is that the eigenfunction to the original problem is lost. The solution along the complex contour $(u[f(x)])$ cannot be used to

generate the solution along the real y-axis. However, for many problems in mathematical physics it is the eigenvalue which is of primary interest, and so this difficulty may not arise.

The Quadratic Map

The simplest polynomial complex map which avoids a single critical point is the quadratic map

$$y = f(x) = x - P(x^2 - 1), \qquad (5)$$

where $P = P_r + iP_{im}$ is the map parameter. This map was first investigated by Boyd [5] and is the most general quadratic map with fixed points at ± 1. In the case of a single critical point y_c, the transformed differential equation is singular at

$$x_c = x_\pm = \frac{1 \pm \sqrt{1 - 4Py_c + 4P^2}}{2P}.$$

That is, the transformed problem has, in general, two distinct critical points. The error in the pseudospectral approximation to the solution is again geometric, but with δ given by $\delta = \min\{\delta(x_\pm)\}$. The parameter P should be chosen to maximize this value of δ. Gill and Sneddon showed that this can be done by choosing $P = P_{OPT}$, where

$$P_{OPT}[y_c] = \frac{y_c \pm \sqrt{y_c^2 - 1}}{2} \qquad (6)$$

and the sign is chosen so that the contour avoids the branch cut associated with y_c. With this optimum value of P, the two critical points coalesce, leaving $x_+ = x_- = 1/(2P_{OPT})$ and

$$\delta(x_c) = \max\left\{\left|\frac{1 \pm \sqrt{1 - 4P_{OPT}^2[y_c]}}{2P_{OPT}[y_c]}\right|\right\}.$$

There are two comments to be made about this simple result. First, in obtaining the result it was necessary to ignore the algebraic factor in the error term. This means that it is an asymptotic result and may not be applicable for all N. However, to extend the analysis to all N (to find $P_{OPT}[y_c, N]$) would be impractical. Second, the locations of the critical points may not be known *a priori* since they can depend on the unknown eigenvalue. In such cases it may be possible to obtain an approximate value by other means. For example, if the problem is to be solved for a range of parameter values (such as the wavenumber), a "continuation" approach may be used, as described in [1, p. 22].

For a real critical point with a banch cut in the upper

TABLE I

Optimal Quadratic Map Results for a Single Real Critical Point

y_c	P_r	P_{im}	δ
0.0	0.000	−0.500	2.414
0.2	0.100	−0.490	2.397
0.4	0.200	−0.458	2.342
0.6	0.300	−0.400	2.236
0.8	0.400	−0.300	2.040
0.90	0.450	−0.218	1.859
0.95	0.475	−0.156	1.704
0.99	0.495	−0.070	1.444

half-plane, the optimal P and δ values are presented in Table I for various locations of the critical point. Quite large δ values are obtained when the critical point is near the center of the interval $[-1, 1]$, but these decrease markedly for near-boundary critical points. This is a result of the requirement that the new contour passes through the end-points so that the boundary conditions may be applied. It is this latter type of singularity that is of particular interest in this paper.

3. COMPOSITE MAPS

For those cases where the improvement in δ is not great, or perhaps even when it is, another complex map could be applied to the transformed problem, treating it as the original problem. This could be achieved with $x = g(z)$, where g is a complex map so that now $y = f \circ g(z) = f[g(z)]$ and $\delta(z_c) > \delta(x_c)$. One could envisage applying several such complex maps to increase δ indefinitely. However, in general there are two main drawbacks to this. First, for problems with more than one critical point, the number of transformed critical points grows rapidly with the level of composition. This in turn can increase the degree of the individual polynomial maps needed at each stage. Second, the calculations needed to carry out each transformation soon become very tedious. In the case of a single critical point, however, these difficulties do not arise since the optimal quadratic map yields a single transformed critical point at each stage. Also, explicit formulae can be generated for composite quadratic complex maps in that case.

For the optimal quadratic map with P given by (6),

$$\begin{aligned} y &= x - P_{OPT}[y_c](x^2 - 1) \\ &= y_c - P_{OPT}[y_c](x - x_c)^2, \end{aligned} \qquad (7)$$

where the single transformed critical point is given by

$$x_c = \frac{1}{2P_{OPT}[y_c]}.$$

If the optimal quadratic map is similarly applied for $x = g(z)$, then

$$x = x_c - P_{OPT}[x_c](z - z_c)^2, \qquad (8)$$

where now

$$P_{OPT}[x_c] = \frac{x_c \pm \sqrt{x_c^2 - 1}}{2}, \quad z_c = \frac{1}{2P_{OPT}[x_c]}$$

and

$$\delta(z_c) = \max\left\{\left|\frac{1 \pm \sqrt{1 - 4P_{OPT}^2[x_c]}}{2P_{OPT}[x_c]}\right|\right\}.$$

Substituting (8) into (7) yields the two-level composite map

$$y = y_c - P_{OPT}[y_c]P_{OPT}^2[x_c](z - z_c)^4.$$

This result easily generalizes to the p level composite map

$$y = f_p(x) = y_c - P(x - x_c^{(p)})^{2^p}, \quad p \geq 1, \qquad (9)$$

where

$$P = \prod_{j=1}^{p} P_j^{2^{j-1}}, \quad P_j = \frac{x_c^{(j-1)} \pm \sqrt{(x_c^{(j-1)})^2 - 1}}{2}, \quad j = 1, ..., p,$$

and

$$x_c^{(j)} = \frac{1}{2P_j}, \quad x_c^{(0)} = y_c.$$

The resulting value of δ is

$$\delta(x_c^{(p)}) = \max\left\{\left|\frac{1 \pm \sqrt{1 - 4P_p^2}}{2P_p}\right|\right\}.$$

To illustrate the potential benefits of these maps, consider the case of a single critical point $y_c = 0.99$. Table II

TABLE II

Composite Quadratic Map Results for a Single Critical Point at $y_c = 0.99$

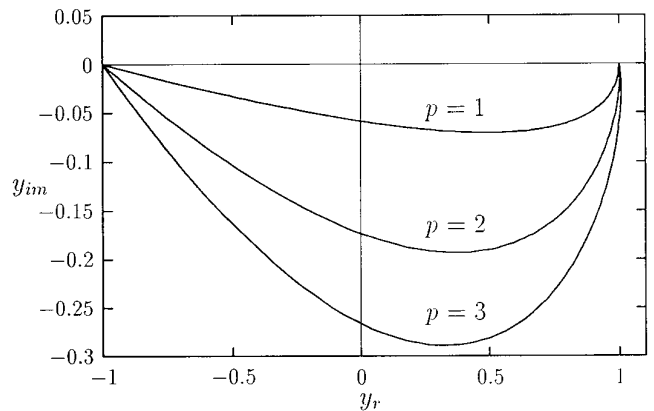| p	P_p	$x_c^{(p)}$	$\delta(x_c^{(p)})$
0	0	0.99	1.00
1	$0.495 - 0.071i$	$0.990 + 0.141i$	1.444
2	$0.321 - 0.130i$	$1.338 + 0.542i$	2.663
3	$0.165 - 0.089i$	$2.346 + 1.262i$	5.230

FIG. 1. Optimal contours in the complex y-plane generated by the one, two, and three level composite quadratic complex maps for a single critical point $y_c = 0.99$.

summarizes the results for the application of one, two and three level composite quadratic maps, and Fig. 1 illustrates the contours generated by these maps. Note that the one level map is the quadratic map and that the application of the higher degree composite maps has the desired effect of "pushing" the transformed critical point even further from the interval $[-1, 1]$. With $N = 10$ terms in the pseudo-spectral approximation, the error with the quadratic map should in theory be roughly $1.444^{-10} \sim 10^{-2}$, or 1%. With the same discretization, the errors for the two and three level maps should be roughly 10^{-4} and 10^{-7}, which are significant improvements indeed. It can also be shown that for large values of p, the value of δ approximately doubles at each level. In view of this, the potential of these composite maps for single critical points (whether they are near a boundary or not) appears to be considerable. However, it will be shown that, in practice, this is not always the case and one may have to be content with the improvement obtained in using the quadratic map.

It should also be noted that the maps (9) can be seen as special cases of the family of higher degree maps given by

$$y = y_c - P(x - x_c)^{2n}$$

for integer values of n. The values of P and x_c can be found from the requirement that $y(\pm 1) = \pm 1$. Higher degree maps were also considered in [1] but for a different purpose. In that paper, the increased number of disposable map parameters allowed a greater increase in the maximum value of δ, particularly when there was more than one critical point. The advantage with the composite quadratic maps for problems with a single critical point is that no optimization of δ needs to be performed manually. The optimal map parameters are given by explicit, analytic expressions.

4. TEST PROBLEM

The pseudospectral method, combined with the composite quadratic maps, is used to solve the problem

$$(y - y_c)^2 u''(y) + [1 - \lambda(y - y_c)^2]u(y) = 0, \quad (10)$$

subject to

$$u(-1) = u(1) = 0, \quad (11)$$

where y_c is the single critical point and λ is the eigenvalue sought. Since our interest is in problems with near-boundary critical points, consider the above problem with $y_c = 0.99$. Equation (10) is actually a generalization of a problem considered in [1]. The analytic solution is known and the solution satisfying (11) is

$$u(y) = B\sqrt{y - y_c}\{J_{i\sqrt{3}/2}[i\sqrt{\lambda}(y - y_c)] + \gamma J_{-i\sqrt{3}/2}[i\sqrt{\lambda}(y - y_c)]\}, \quad (12)$$

where B is an arbitrary constant. In Eq. (12), $J_\nu(y)$ is the Bessel function of the first kind of order ν, the constant γ is given by

$$\gamma = \frac{J_{i\sqrt{3}/2}[i\sqrt{\lambda}(1 - y_c)]}{J_{-i\sqrt{3}/2}[i\sqrt{\lambda}(1 - y_c)]},$$

and λ is a solution of

$$J_{i\sqrt{3}/2}[i\sqrt{\lambda}(1 - y_c)]J_{-i\sqrt{3}/2}[i\sqrt{\lambda}(-1 - y_c)]$$
$$- J_{i\sqrt{3}/2}[i\sqrt{\lambda}(-1 - y_c)]J_{-i\sqrt{3}/2}[i\sqrt{\lambda}(1 - y_c)] = 0. \quad (13)$$

The algebraic package Mathematica can be used to calculate the eigenvalue of smallest magnitude by solving the transcendental equation (13). To 16 decimal places this is

$$\lambda_1 = -1.1901285054724449 - 1.6418523354678106i.$$

The method was coded in Fortran 77 and run on an RS6000 workstation employing double precision arithmetic. The generalized matrix eigenproblem which results was solved using the IMSL routine DGVLCG. The relative errors in λ_1 obtained by the pseudospectral method with these composite maps are plotted against the matrix size
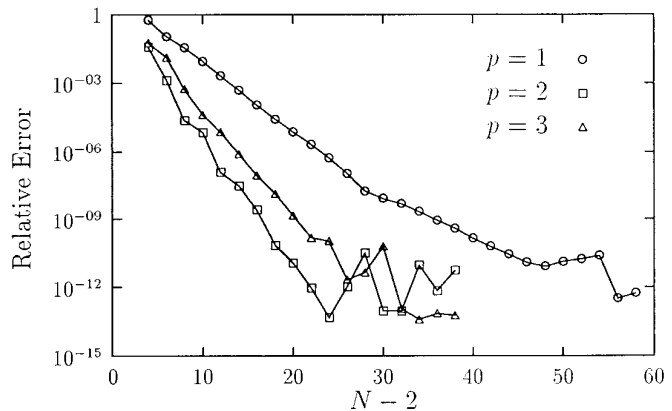

FIG. 2. Convergence of the one, two, and three level composite quadratic maps combined with the pseudospectral method for (10) and (11). Plotted are the relative errors (in logscale) as functions of $N - 2$.

$(N - 2)$ for various values of N in Fig. 2. Approximate geometric convergence is obtained with all three maps. The application of the two level composite map with the pseudospectral method yielded a much faster rate of convergence, as suggested by the larger theoretical δ value in Table II. However, the three level map did not perform as well as the two level map, but produced relative errors between those of the one and two level maps. This is contrary to the theoretical results anticipated from Table II and requires further investigation.

The result that $E \sim \delta^{-N}$ is an asymptotic result and so it may not be indicative of the error for small to moderate N. Since the results for the two and three level maps already appear to be affected by round-off, it is not practical to check this by solving the problem with larger values of N. However, an alternative approach may be taken since the eigenfunction is known analytically.

The series truncation error in an N term pseudospectral solution to a differential equation is of the order of the last retained coefficient of the Chebyshev series approximation to the eigenfunction—i.e., $E_S = O(|a_N|)$. Here, the eigenfunction is the transformation of (12) under the map (9) for the three composite maps given in Table II. The high precision available in Mathematica can be used to calculate $|a_N|$ for any value of N. A plot of $|a_N|$ versus $N - 2$ for each composite map should then reflect the convergence observed in Fig. 2, but without the influence of round-off errors. The results are given in Fig. 3 and are consistent with the results of Fig. 2 for $N < 25$. However, for $N - 2 \geq 65$ the three level composite map does produce Chebyshev coefficients with magnitude less than those produced by the two level composite map, as expected from the theoretical (asymptotic) results. However, the modulus of the Chebyshev coefficients (and therefore the relative errors) at this "cross-over" point are of the order of 10^{-30}. In practice this accuracy is rarely sought or achieved on
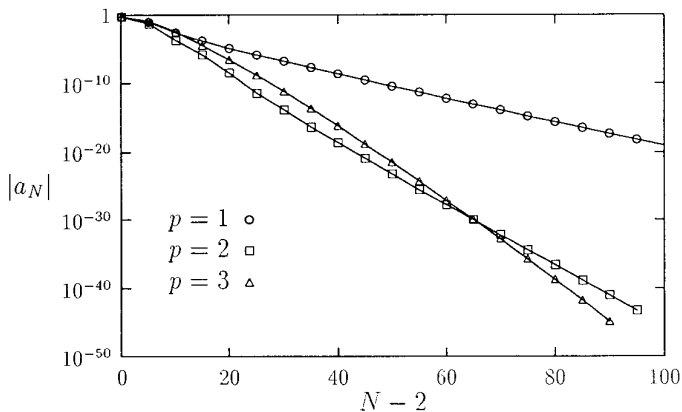
FIG. 3. Magnitude of the exact Chebyshev coefficients as functions of $N - 2$ of the transformed eigenfunction (12) under the one, two, and three level composite quadratic maps.

finite precision computers (as evident in Fig. 2). These results highlight that, while the asymptotic theory may be used as a guide, in practice the values of N for which the theory is valid may be too large or imply the error is far smaller than normally required.

A likely explanation for the discrepancy between experiment and the predictions of Table II for moderate values of N is that Table II does not include the effects of the algebraic factors in the formula for the error. These factors are often omitted on the basis that the geometrically decreasing factor dominates as $N \to \infty$. Also this simplification is needed in order to obtain formulae such as (6) for the optimal map parameters. In practice, however, a finite value of N is used and it may be the case that previously discarded algebraic factors have some influence on the rate of convergence.

These ideas can be confirmed by considering the Chebyshev expansion of the transformation of a known function such as $u(y) = (y - y_c)^{-1}$ which has a simple pole at $y = y_c$. Under the composite map (9), the function to be approximated is

$$v(x) \equiv u[f_p(x)] = \frac{-1}{P(x - x_c^{(p)})^{2^p}},$$

which has a pole of order 2^p at $x_c^{(p)} = f_p^{-1}(y_c)$. The Chebyshev coefficients for $v(x)$ are given in closed form in Elliot [10]. It follows that, since $E \sim |a_N|$ as $N \to \infty$,

$$E_p \sim N^{2^p-1}[\delta(x_c^{(p)})]^{-N} \quad \text{as } N \to \infty, \qquad (14)$$

where p is the level of composition. The increase in the order of the pole to 2^p is reflected in the algebraic factor N^{2^p-1} in the expression for the error. For example, with $p = 3$ and $N = 20$, the algebraic factor is of the order of

10^9. The composite map will be beneficial only if the increase in δ is sufficient to overcome the increase in the algebraic factor.

In this case, a rough test can be constructed to determine what level of composition should be used. For a given discretization, $N = N_*$, a p level composite map will be an improvement over the $(p - 1)$ level map only if $E_p < E_{p-1}$. Using (14) this leads to the requirement that

$$\left(\frac{\delta_p}{\delta_{p-1}} \right)^{N_*} > N_*^{2^{p-1}}.$$

If δ_p/δ_{p-1} is given its limiting value of 2, we need $N_* > 2^{p-1} \log_2 N_*$ or

$$p < 1 + \log_2 N_* - \log_2(\log_2 N_*)$$

for the p level map to be an improvement. This suggests that the three level map will be unsuitable for $N \le 15$ and the four level map will be unsuitable for $N \le 40$. This simple analysis indicates that, for finite values of N, algebraic factors will play a role in determining the effectiveness of composite quadratic maps.

5. CONCLUSIONS

In this paper the numerical solution of singular, second-order linear differential eigenproblems by pseudospectral methods was considered. In particular, the case of a single critical point near an endpoint of the (finite) computational domain was investigated. Such situations are often fatal for standard numerical techniques and the improvement that a quadratic complex map produces can also be limited.

Composite complex maps offer a means of overcoming this problem. While the theoretical results indicated significant improvements in the rate of convergence of the numerical method, in practice only partial success resulted. The discrepancy was a result of neglecting algebraic factors in the formula for the error in order to obtain simple expressions for the optimum map parameters. Despite this, a measurable degree of improvement was obtained for the test problem. The two level composite quadratic map was significantly more accurate than the quadratic map. For example, with $N = 10$, the composite map was 1000 times more accurate.

One disadvantage with composite complex maps is that they may be difficult to implement in the case of multiple critical points. The optimal map parameters cannot be provided explicitly, and the degree of the map at each level of composition can grow rapidly. Even so, the results for a single critical point provide a useful insight into the properties of complex mapping methods.

ACKNOWLEDGMENTS

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