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An Analytical and Numerical Study of the Two-Dimensional Bratu Equation

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Bratu's problem, which is the nonlinear eigenvalue equation $\Delta u + \lambda \exp(u) = 0$ with $u = 0$ on the walls of the unit square and λ as the eigenvalue, is used to develop several themes on applications of Chebyshev pseudospectral methods. The first is the importance of *symmetry*: because of invariance under the C_4 rotation group and parity in both x and y, one can slash the size of the basis set by a factor of eight and reduce the CPU time by three orders of magnitude. Second, the pseudospectral method is an *analytical* as well as a numerical tool: the simple approximation $\lambda \approx 3.2A \exp(-0.64A)$, where A is the maximum value of $u(x, y)$, is derived via collocation with but a single interpolation point, but is quantitatively accurate for small and moderate A. Third, the Newton–Kantorovich/Chebyshev pseudospectral algorithm is so efficient that it is possible to compute good numerical solutions—five decimal places—on a *microcomputer* in BASIC. Fourth, asymptotic estimates of the Chebyshev coefficients can be very misleading: the coefficients for moderately or strongly nonlinear solutions to Bratu's equations fall off exponentially rather than algebraically with v until v is so large that one has already obtained several decimal places of accuracy. The corner singularities, which dominate the behavior of the Chebyshev coefficients in the *limit* $v \to \infty$, are so weak as to be irrelevant, and replacing Bratu's problem by a more complicated and realistic equation would merely exaggerate the unimportance of the corner branch points even more.

KEY WORDS: Bratu's problem; nonlinear eigenvalue problem; spectral methods.

1. INTRODUCTION

The two-dimensional nonlinear eigenvalue problem known as Bratu's equation has a dual importance. First, it arises in a wide variety of physical

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applications, ranging from chemical reactor theory and radiative heat transfer to the expansion of the universe (Abbot, 1978). Second, because of its simplicity, his equation is widely used to test nonlinear eigenvalue solvers (Bank and Chan, 1986).

The problem is defined by

$$u_{xx} + u_{yy} + \lambda e^u = 0 \tag{1}$$

on the square $[-1, 1] \times [-1, 1]$ subject to the boundary condition

$$u = 0 \qquad \text{on all four walls} \tag{2}$$

where λ is the eigenvalue. Most other references pose the problem on the unit square $[0, 1] \times [0, 1]$, but the only effects of this are to (1) require relabeling the axes of plots of $u(x, y)$ without changing the shape and (2) multiply our values of λ by a factor of 4.

Following Abbott (1978), we measure the amplitude of $u(x, y)$ by its value at the center of the square, which turns out to be the maximum of the function

$$A \equiv u(0, 0) = \|u\|_\infty \tag{3}$$

Previous work has shown that Bratu's problem has but a single branch of solutions for all positive A.

This new study of an old equation has two purposes. First, because of the intrinsic importance of Bratu's problem, it is useful to offer some new graphs and tables to fill in the gaps of earlier investigations. The second goal is to use Bratu's equation as a test for a hierarchy of both analytical and numerical applications of the pseudospectral method to multidimensional eigenvalue problems. We will find that this family of techniques is extremely successful in spite of the absence of such trendy devices as multigrid, preconditioned iterations, and pseudo-arclength continuation.

In the next section, we briefly explain how the high symmetry of the problem allows one to reduce the total number of pseudospectral basis functions by a factor of eight from what would be needed to achieve a given accuracy if the symmetries were ignored. Section 3 explains how collocation with just *one* basis function at *one* interpolation point gives an *analytic* solution to this *two-dimensional, nonlinear* eigenvalue problem, which is nonetheless accurate to within a few percent for all amplitudes up to the limit point where $\lambda(A)$ is a maximum. Section 4 derives an improved analytic solution by a perturbative simplification with three-degree-of-freedom collocation. Section 5 describes a Chebyshev polynomial/Newton–Kantorovich numerical algorithm that is very accurate even for strongly nonlinear solutions. The method was so effective that all calculations were

done on a microcomputer using ordinary Gaussian elimination for the final, rate-determining step. Section 6 discusses the "corner" singularities and how they can be resolved if very high accuracy is needed. The article ends with a summary and prospectus. A few programming notes are collected in the Appendix.

2. SYMMETRY

When the solution is known to have some particular symmetry property, this is a great boon to the application of the pseudospectral method (or Galerkin's method) because the equation can be solved using a *restricted* basis set, which retains only those basis functions that have the *same symmetry* as the solution. The proof is given in many books on applications of group theory to quantum mechanics, such as Merzbacher (1970) and Cotton (1963).

The solution of Bratu's equation is symmetric about the origin in both x and y. Consequently, only the even-degree Chebyshev polynomials are needed to construct the appropriate two-dimensional basis functions. For a given resolution, this double parity reduces the size of the basis set by a factor of four.

However, if we rotate the square through an angle of 90°, neither the differential equation nor the boundary conditions are altered. Thus, the solution is also, in the language of group theory, "invariant under the rotation group C_4," which is the group of rotations through any integral multiple of 90°. In Section 5, we explicitly construct a basis set whose elements, formed as sums of $T_m(x)\,T_n(y)$ for various m and n, are symmetric in both x and y and invariant under the C_4 rotation group.

The payoff is to reduce the total number of basis functions (for a given desired accuracy) by a factor of eight. This is turn reduces the required memory by a factor of 64 (since pseudospectral matrices are dense) and the execution time by a factor of 512 (since Gaussian elimination is used to solve the needed linear equations).

The hardest task is to recognize that a problem has certain symmetries. The author knows of no simple *a priori* proof that the solution of Bratu's equation has the invariance properties described above. It is quite easy, however, to show that these symmetries are at least plausible in the sense that (1) and (2) are both invariant under $\pi/2$ rotations, so that it is reasonable that $u(x, y)$ might have the same property.

The best strategy is to guess the symmetries of $u(x, y)$ and then determine *a posteriori* if the guess is correct. If the computed solution gives a large residual when substituted into the original differential equation, then at least some of the hoped-for symmetries are missing, and one must try

again with a larger basis set. So long as one is careful to check the residuals, as described further in Section 5, one can safely exploit the full invariance properties of a problem even when it is not possible to prove these invariance properties in advance.

3. THE SIMPLEST ANALYTIC SOLUTION: ONE-POINT COLLOCATION

The pseudospectral method, also known as "orthogonal collocation," is thoroughly described along with its older cousin, Galerkin's method, in the monographs of Finlayson (1972) and Gottlieb and Orszag (1977). The first step is to assume that the unknown $u(x, y)$ can be expanded as a series of spectral basis functions

$$u = \sum_{n=1}^{N} a_n \phi_n(x, y) \tag{4}$$

where the $\phi_n(x, y)$ are chosen to (1) have the property of completeness, so that the error decreases to 0 as $N \to \infty$, and (2) satisfy the boundary conditions. Substituting (4) into the differential equation then defines the so-called *residual*, $R(x, y; \lambda, a_1, a_2, ..., a_N)$. If the truncated series were the exact solution, the residual function would be identically zero, so the goal of all series expansion methods is to impose constraints that minimize the residual and can be solved for the spectral coefficients a_n. Galerkin's method and the pseudospectral method differ only in the sense in which the residual is minimized.

The pseudospectral constraints are that the residual should be exactly zero at N discrete "interpolation" or "collocation" points, that is,

$$R(x_i, y_i; \lambda, a_1, a_2, ..., a_N) = 0, \qquad i = 1, ..., N \tag{5}$$

The most effective choice of interpolation points is to pick both x_i and y_i to be the roots of an orthogonal polynomial of the same family as that used to construct the basis functions. When tensor products of Chebyshev polynomials are combined to create $\phi_n(x, y)$ as done in Section 5, for example, the interpolation points are roots of the Chebyshev polynomials, too.

Finlayson (1972) points out, however, that although Chebyshev polynomials are the best basis for *high-resolution numerical* computation, they are not optimum when orthogonal collocation is applied with a handful of points to generate a *crude* but *analytic* approximation. The reason is that the Chebyshev polynomials weight the whole interval

$[-1, 1]$ equally and give a very uniform approximation to an arbitrary function $u(x, y)$. However, the solution of Bratu's equation is *not* arbitrary, because the boundary conditions determine its behavior near the walls: u must tend to zero as any of the boundaries is approached. Therefore, we want an approximation that stresses the *center* of the domain. This suggests a set of interpolation points that are closer to the origin than their Chebyshev counterparts.

Finlayson describes a systematic procedure for choosing such points. The Chebyshev polynomials are part of a larger family known as the Gegenbauer polynomials, which are orthogonal on $[-1, 1]$ with respect to the weight function $w(x) \equiv (1-x^2)^b$, where $b = -1/2$ gives the Chebyshev polynomials themselves. The larger b is, the more strongly the Gegenbauer polynomials favor the center of the interval at the expense of what would be higher errors near the endpoints were it not for the boundary conditions. Finlayson recommends $b = 1$, and this is the choice made here and in the next section.

With just a single degree of freedom, the collocation point is

$$(x_1, y_1) = (0.447, 0.447) \tag{6}$$

where 0.447 is an approximation to $(1/5)^{1/2}$. The corresponding Chebyshev point is (0.707, 0.707), which gives an error in the maximum value of λ that is nine times larger than what is obtained via (6).

The most obvious choice of interpolation point, of course, is the center of the square, but this gives roughly three times the error of (6). The reason is that because of the high symmetry of the solution and the basis functions, imposing the condition that the residual function is zero at one point away from the origin guarantees that the residual also vanishes at $(\pm x_1, \pm y_1)$, so that our one-point approximation is effectively a four-point approximation.

The lowest basis function that (1) is a polynomial and (2) vanishes at the four sides of the square gives

$$u(x, y) \approx A(1-x^2)(1-y^2) \qquad \text{[1-point approx.]} \tag{7}$$

Substituting this into the differential equation gives

$$R(x, y; \lambda, A) \equiv -4A + 2Ax^2 + 2Ay^2 + \lambda \exp[A(1-x^2)(1-y^2)] \tag{8}$$

Since the approximation (7) automatically satisfies the boundary conditions, our sole task is to determine A so that the residual is as small as possible. The condition

$$R(0.447, 0.447; \lambda, A) = 0 \tag{9}$$

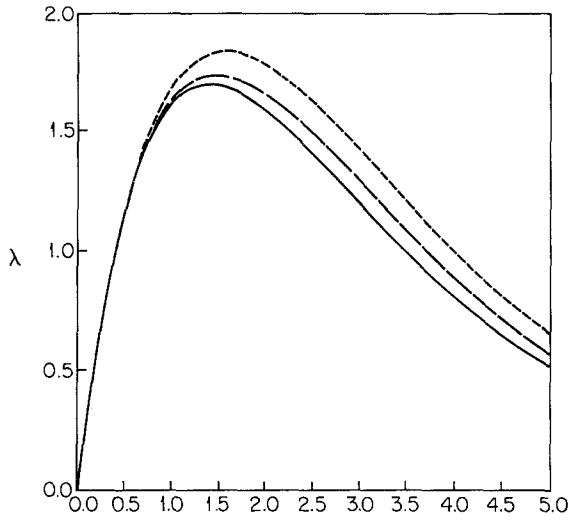

Fig. 1. (—) The eigenvalue $\lambda(A)$ as given by numerical integration, compared with (— —) the three-basis function approximation derived in Section 4 and (– –) the one-collocation point analytic approximation (10).

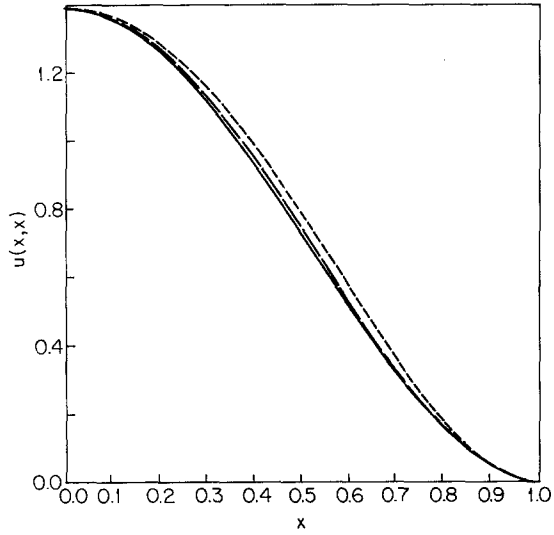

Fig. 2. The function $u(x, x)$—that is, $u(x, y)$ along the diagonal of the square domain—displayed for $A = 1.39$ [the limit point where $\lambda(A)$ is largest] as calculated through three different means. The comparison is between (—) a high-resolution Chebyshev pseudospectral calculation, (– –) the three-point pseudospectral approximation, and (— —) the one-basis-function analytic formula, $u(x, y) \approx A(1 - x^2)(1 - y^2)$. The maximum absolute errors are 0.017 and 0.06, respectively. Because of the symmetry with respect to the origin, only $x \geqslant 0$ is graphed.

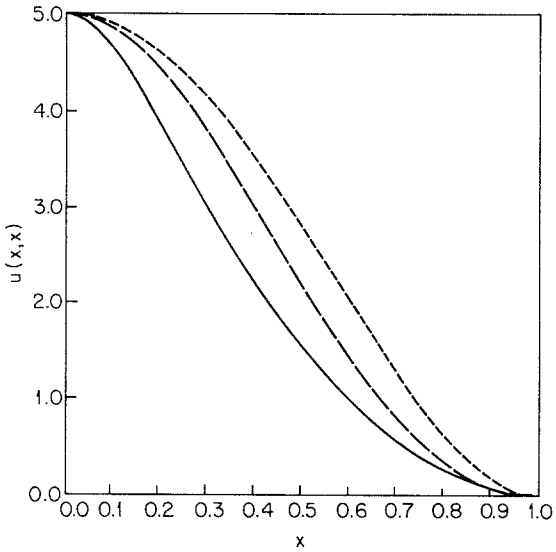

Fig. 3. Identical with Fig. 2, except for $A = 5$ (strong nonlinearity). The maximum absolute errors are 1.30 for the one-point approximation and 0.81 for the three-basis-function sum. As explained in Section 6, $u(x, y)$ is weakly singular at the corners, so making comparisons along a slice of the domain that includes the corners is a severe test of the approximations that are compared with the exact solution (solid curve).

gives the analytic approximation

$$\lambda \approx 3.2Ae^{-0.64A} \qquad \text{[1-point eigenvalue approx.]} \tag{10}$$

Figure 1 compares the accuracy of (10) (and the improved analytic approximation derived in the next section) with the exact $\lambda(A)$. Figures 2 and 3 compare (7) with the exact $u(x, y)$ along the diagonal $x = y$ for two different values of A. Table I compares the exact values of λ and A at the limit point [which is defined to be where $\lambda(A)$ is a maximum] with those

Table I. A Comparison of the Exact Limit Point [Defined to be where $\lambda(A)$ Is a Maximum] with the Predictions of the One-Point and Three-Point Approximations

Formula	λ_{max}	Relative error, %	A_{limit}	Relative error, %
Exact	1.702	—	1.39	—
One-point	1.84	8.0	1.56	12.4
Three-point	1.735	1.9	1.465	6.3

of the analytic approximations. Although the approximation (7) plus (10) is very simple, the accuracy is remarkably good. Equation (10) correctly reproduces the qualitative behavior of $\lambda(A)$ for *all* A. Even at the limit point, the relative error is only about 7.5%.

Finlayson (1972) is full of similar examples; the pseudospectral method is often so accurate for simple, idealized problems that a one- or two-point approximation is sufficient. When this is true, the residual conditions can be solved to give an explicit, analytic solution.

4. THREE-POINT COLLOCATION: AN IMPROVED ANALYTIC APPROXIMATION

The refined solution given in this section is similar to the one-degree-of-freedom approximation derived above except that the basis includes three functions:

$$u(x, y) \approx (1-x^2)(1-y^2)[A + B(x^2+y^2) + Cx^2y^2] \tag{11}$$

Note that the factor outside the brackets guarantees that the approximation vanishes at the boundaries. All the basis functions are invariant under the substitutions $x \to (-x)$ (even parity in x), $y \to (-y)$ (even parity in y), and $x \to y$ and $y \to x$ (rotation through 90°).

The corresponding collocation points are

$$\begin{aligned} &(x_1, y_1) = (0.285, 0.285) \\ &(x_2, y_2) = (0.285, 0.765) \qquad \text{[interpolation points]} \\ &(x_3, y_3) = (0.765, 0.765) \end{aligned} \tag{12}$$

where 0.285 and 0.765 are the two positive roots of the fourth-degree Gegenbauer polynomial. By demanding that the residual function, obtained by substituting (11) into (1), should vanish at these three collocation points, we obtain three equations in three unknowns. Because of all the symmetries, the residual function is zero not only at the three points (12), but also at (0.765, 0.285) and the 12 points that are the images of these four points under rotations through an integer multiple of 90°—16 points in all.

The three nonlinear algebraic equations that results from the pseudospectral method are too complicated to solve in closed form, but two simplifications are possible. First, if we take the lowest spectral coefficient A as a parameter so that the eigenvalue λ and the higher spectral

coefficients are the unknowns, then the three residual constraints are *linear* in λ. Arbitrarily choosing to solve the constraint at (x_2, y_2) gives

$$\lambda = (2.667A + 4.83B + 0.127C)\exp(-0.381A - 0.254B - 0.018C) \tag{13}$$

which is the first simplification.

The two remaining constraint equations become

$$(2.667A + 4.83B + 0.127C)\exp(0.463A - 0.117B - 0.013C) - 3.675A + 1.582B + 0.153C = 0 \tag{14a}$$

$$(2.667A + 4.83B + 0.127C)\exp(-0.209A - 0.053B + 0.041C) - 1.659A - 5.138B - 2.439C = 0 \tag{14b}$$

These two equations are still too complicated to solve in closed form as they are, but note that the spectral coefficients B and C appear in the exponentials in (14a) and (14b) only with small numerical coefficients. If we drop them—only from the exponentials and without approximating any term involving the known parameter A—then (1a) and (14b) are linearized, and their solutions are

$$B = A(0.829 - 0.566e^{0.4630A} - 0.0787e^{-0.209A})/G \tag{15a}$$

$$C = A(-1.934 + 0.514e^{0.4630A} + 1.975e^{-0.209A})/G \tag{15b}$$

where the denominator of both $B(A)$ and $C(A)$ is

$$G \equiv 0.2763 + e^{0.4630A} + 0.0483e^{-0.209A} \tag{15c}$$

With this second simplification, (13) and (15a)–(15c) describe an approximation that is no longer a simple pseudospectral solution, but rather a collocation-cum-perturbation approximation. Nonetheless, Figs. 1–3 show that it is considerably more accurate [for $\lambda(A)$, at least twice as good] as the single-degree-of-freedom formulas derived in the previous section.

The algebraic manipulation language REDUCE was used to streamline the algebra needed to compute (13) and (15a)–(15c). With this tool or a similar language like MACSYMA, it is straightforward to derive explicit analytic approximations of considerably greater complexity, i.e., more interpolation points and a higher approximation to the solution of the nonlinear residual constraint equations. We shall stop with the three-point approximation, however, and turn to high-resolution numerical calculations instead.

5. THE CHEBYSHEV PSEUDOSPECTRAL/NEWTON–KANTOROVICH METHOD

To achieve high accuracy—or even a coarse approximation for large amplitude—one must resort to purely numerical computation. The first task is to choose pseudospectral basis functions appropriate for the boundary conditions and the symmetry of the problem.

First step: since the boundary conditions are not periodic, the building blocks for the basis functions will be Chebyshev polynomials in x multiplied by Chebyshev polynomials in y. As noted above, Gegenbauer polynomials are more efficient for low-order *analytic* calculations, but Chebyshev polynomials are both easier to program and more accurate when the number of basis functions is large.

Second step: since $u(x, y)$ is symmetric with respect to the origin in both x and y, we should restrict the basis to functions with this same double parity. Thus, the tensor products of Chebyshev polynomials will be restricted to terms of even degree like $T_{2m}(x)\,T_{2n}(y)$, where m and n are integers.

Third step: to force each basis function to satisfy *individually* the homogeneous boundary conditions, we alter the building blocks to

$$\phi_{m,n} \equiv [T_{2m}(x) - 1][T_{2n}(y) - 1], \qquad m = 1, 2,...; \quad n = 1, 2,... \tag{16}$$

Since $T_{2n}(\pm 1) = 1$ for all integral m, it follows that $\phi_{mn}(x, y) = 0$ wherever either $|x| = 1$ or $|y| = 1$, i.e., on all four sides of the unit square.

Fourth step: because of the C_4 rotational symmetry, we may further restrict the basis set to combinations that are invariant under the replacement of x by y and y by x. The simplest such basis functions are defined by

$$\begin{aligned} A_{mn} &\equiv [\phi_{mn}(x, y) + \phi_{nm}(x, y)] && m < n; \quad n = 1, 2,... \\ &= \phi_{mn}(x, y) && m = n; \quad n = 1, 2,... \end{aligned} \tag{17}$$

If a "square" truncation is applied to the original basis functions (16)—that is, only those elements with $m \leqslant v$ and $n \leqslant v$ are kept—then taking the rotationally invariant combinations of (17) reduces the total number of basis functions to

$$N = v(v + 1)/2 \qquad \text{["triangular truncation"]} \tag{18}$$

and this "triangular" truncation will be used in all the numerical calculations described here.

The fifth and final step is cosmetic but useful. The easiest way to

specify an amplitude parameter A is to choose it to be equal to the coefficient of the lowest basis function, $\phi_{22}(x, y)$. In the analytic approximations of the previous two sections, this was a very convenient choice because all the other basis functions vanish at the origin, where $u(x, y)$ is a maximum, so that A also could be interpreted as $\|u\|_\infty$, the norm of $u(x, y)$. We can retain this interpretation for the high-resolution numerical calculations by setting

$$\phi_{22}(x, y) \equiv \tfrac{1}{4}[T_2(x) - 1][T_2(y) - 1] \tag{19a}$$

$$\phi_{mn}(x, y) \equiv A_{mn}(x, y) - A_{mn}(0, 0)\,\phi_{22}(x, y), \qquad m \leqslant n \tag{19b}$$

where (19a) ensures that $\phi_{22}(0, 0) = 1$ and (19b) guarantees that $\phi_{mn}(0, 0) = 0$ unless both m and n equal two.

The interpolation points are tensor products of the roots of Chebyshev polynomials, that is,

$$x_i = \cos[\pi(2i - 1)/4v], \qquad y_j = \cos[\pi(2j - 1)/4v]$$
$$i \leqslant j; \qquad j = 1, 2, \ldots, v \tag{20}$$

The restriction $i \leqslant j$ is consistent with the "triangular" truncation of the basis functions: because of the symmetries, all the interpolation points lie in a triangle that occupies but one-eighth the rea of the unit square.

In a similar way, the total number of basis functions is only one-eighth that of the full collection of products of Chebyshev polynomials with $m = 1, \ldots, 2v$ and $n = 1, \ldots, 2v$. Since the pseudospectral method generates full matrices and we choose to solve the corresponding linear algebra problems via Gaussian elimination without special tricks, this reduction in basis functions through symmetry translates into a reduction of 1/64 in memory storage and 1/512 in operation count.

The Newton–Kantorovich method (Birkhoff and Lynch, 1984) was used to reduce the nonlinear differential equation to an iteration that requires solving only a linear boundary value problem at each step. The first step is to make the substitutions

$$\begin{aligned} u(x, y) &\to u(x, y) + \Delta(x, y) \\ \lambda &\to \lambda + \delta \end{aligned} \tag{21}$$

into the differential equation to obain, without approximation,

$$(\Delta_{xx} + \Delta_{yy}) + u_{xx} + u_{yy} + \lambda z^{u+\Delta} + \delta e^{u+\Delta} = 0 \tag{22}$$

If we now identify $u(x, y)$ and λ with the current iterates and $\Delta(x, y)$ and δ

as small corrections, expand (22) about $u(x, y)$ and δ, and then discard terms in Δ^2 and $\Delta\delta$, we obtain the iteration

$$\begin{gathered} \Delta_{xx}+\Delta_{yy}+\lambda^{(i)}\exp(u^{(i)})\Delta+\exp(u^{(i)})\delta=-[u_{xx}^{(i)}+u_{yy}^{(i)}+\lambda^{(i)}\exp(u^{(i)})] \\ u^{(i+1)}=u^{(i)}+\Delta, \qquad \lambda^{(i+1)}=\lambda^{(i)}+\delta \end{gathered} \tag{23}$$

and repeat. For notational simplicity, we have suppressed the superscripts on Δ and δ, but these corrections must be computed by solving a linear differential equation at each iteration.

This procedure is associated with Newton's name because its strategy is similar to that of the ordinary Newton's method for solving algebraic equations: linearize the nonlinear function via a first-order Taylor expansion and solve the linear equation to obtain a correction. Kantorovich showed that this idea could be extended to functionals. Technically, the generalized power series expansion requires evaluating a so-called Frechet derivative, but one can obtain the same result by multiplying Δ and δ by a dummy scalar parameter ε and then Taylor expanding in ε.

One unavoidable drawback of the Newton–Kantorovich method is that it requires a good first guess, but this can always be obtained via the so-called "continuation" method—beginning with a known solution and then marching in small steps in a parameter. Here, the amplitude A $[\equiv u(0, 0)]$ is a natural marching parameter. The continuation method can be initialized for small A by using the analytic approximations derived in previous sections.

In point of fact, the analytic approximations work so well so that continuation is unnecessary unless A is large. A first guess consisting of (1) λ based on the one-point formula and (2) $a_i=0$ for all $i\geqslant 2$ was good enough for convergence for A as large as 4. The range of direct solutions can be extended to 5 by applying the UL factorization on every iteration (instead of just the first) and to $A=6$ by using the λ's given by the three-point approximation.

Equation (23) is an unconventional boundary value problem in the sense that it contains a scalar unknown, the eigenvalue correction δ, in addition to $\Delta(x, y)$. The extra degree of freedom allows us to force the coefficient of the lowest basis function to be A. In a standard boundary value problem, δ would be the parameter and A the unknown (along with all the higher spectral coefficients), but it is quite legitimate to have δ and A switch roles.

The reward for taking the eigenvalue as an unknown is that $\lambda(A)$ is single-valued, whereas the inverse function $A(\lambda)$ is double-valued. The point where λ is a maximum is a "limit point" for $A(\lambda)$: $dA/d\lambda=\infty$ at $\lambda=\lambda_{\text{limit}}=1.702$. Ordinary continuation by marching in small steps in λ

will fail utterly in the vicinity of a limit point. Sophisticated variants such as pseudo-arclength continuation (Bank and Chan, 1986) allow one to turn the corner at the limit; Bratu's equation is popular as a test of nonlinear eigenvalue solvers in part precisely because it has a limit point. In the present instance, however, there is much simpler way to deal with the limit point: exchange the roles of λ and A. This method of "parameter exchange" has also been successful in other applications (e.g., Boyd, 1986a).

The pseudospectral solution of (23) is obtained by writing

$$A(x, y) = \sum_{i=2}^{N} d_i \phi_i(x, y) \tag{24}$$

[the sum begins with $i=2$ because the correction to the coefficient of $\phi_1(x, y)$ is zero], where $N = v(v+1)/2$ as in (18); we have condensed two indices, m and n, into a single index with a wider range for notational and programming simplicity. If we write (23) in the abstract form

$$LA + M\delta = R \tag{25}$$

where

$$L \equiv \partial^2/\partial x^2 + \partial^2/\partial y^2 + \lambda^{(i)} \exp(u^{(i)}) \tag{26a}$$

$$M \equiv \exp(u^{(i)}) \tag{26b}$$

$$R \equiv -[u_{xx}^{(i)} + u_{yy}^{(i)} + \lambda^{(i)} \exp(u^{(i)})] \tag{26c}$$

and define a vector of unknowns **a** whose elements are

$$a_1 \equiv \delta, \qquad a_i \equiv d_i, \qquad i = 2, 3, \ldots, N \tag{27}$$

then the usual pseudospectral condition that the truncated solution should exactly satisfy the differential equation at each of N discrete collocation points generates the matrix problem

$$\mathbf{Ha} = \mathbf{r} \tag{28}$$

where

$$H_{i1} \equiv M(x_i, y_i), \qquad H_{ij} \equiv (L\phi_j)|_{x=x_i, y=y_i}$$
$$i = 1, \ldots, N; \qquad j = 2, \ldots, N \tag{29}$$

$$r_i \equiv R(x_i, y_i), \qquad i = 1, 2, \ldots, N \tag{30}$$

In a strict Newton's method, **H** would be recomputed and then factored into the product of an upper triangular matrix with a lower

triangular matrix (UL decomposition) at every iteration. However, because the cost of the factorization is $O(N^3/3)$ while the backsolve is only $O(N^2)$, it is much more efficient to perform the factorization only on the first iteration, and then employ the UL factors of **H** for the first iterate as an approximation to those of the square matrices for all the later iterates. This usually increases the number of iterates, but when N is large, this is a small price to pay for reducing the number of $O(N^3/3)$ steps to one factorization for each nonlinear solution.

When $u(x, y)$ is a smooth function with no singularities on the computational domain, theory predicts that the error as a function of the truncation N should be $O(1)$ and flat until N is large enough to at least crudely resolve the solution and then fall off exponentially fast as N is increased still further. This "exponential" or "infinite-order" convergence is one of the great strengths of spectral methods; finite-difference and finite-element algorithms suffer errors that decrease as *algebraic* functions of N, that is, as $1/N^k$ for some k. Table II shows that the Chebyshev pseudospectral method is quite efficient for this problem.

There is, however, a serious complication: the solution of the differential equation has *branch points* in the four *corners* of the domain that

Table II. Convergence of the Pseudospectral Solution As a Function of N, the Total Number of Two-Dimensional Basis Functions, for Two Different Values of A [$\equiv u(0, 0)$][a]

N	$2v$	λ	Relative error in λ	Maximum error in $u(x, y)$ (divided by A)
$A = 1.39$				
10	8	1.70211	4.6 E−5	6.8 E−4
21	12	1.70203	3.4 E−8	1.5 E−4
36	16	1.70203	3.0 E−8	5.5 E−5
55	20	1.70203	9.8 E−9	1.8 E−5
78	24	1.70203	3.0 E−9	9.0 E−6
$A = 5.0$				
10	8	0.46588	9.8 E−2	6.9 E−2
21	12	0.49676	3.9 E−2	2.0 E−2
36	16	0.51133	1.0 E−2	4.7 E−3
55	20	0.51549	2.3 E−3	1.0 E−3
78	24	0.51648	4.3 E−4	2.2 E−4
Exact		0.51675		

[a] The degree of the highest Chebyshev polynomial in the basis set is also listed.

destroy the exponential convergence for $N \to \infty$—but if four or five decimal place accuracy is adequate, then these corner branch points are probably irrelevant! This subtle but important issue is the theme of the next section.

6. CORNER SINGULARITIES AND MAPPINGS

When the amplitude of $u(x, y)$ is small, the solution is proportional to that of the much-studied linear problem

$$v_{xx} + v_{yy} = -1 \tag{31}$$

with homogeneous Dirichlet boundary conditions on all sides of the square. Birkhoff and Lynch (1984) give a comprehensive review and show that $v(x, y)$ has singularities at the four corners of the domain proportional to

$$r^2 \log r \tag{32}$$

where r is the radial coordinate of a local polar coordinate system centered on a given corner. This is a very weak singularity in the senses that (1) singularities at crack or reentrant corners are much more severe, as reviewed in Birkhoff and Lynch (1984) and (2) second-order finite differences still give an error that is asymptotically $O(h^2)$, where h is the grid spacing, as noted in both Birkhoff and Lynch (1984) and Haidvogel and Zang (1979).

However, the branch points have a severe effect on higher order methods. Fourth-order finite differences give an error that decreases only as $O(h^2)$ and Chebyshev methods give an error that decreases as $O(1/v^4)$, where v is the number of degrees of freedom in each coordinate (Haidvogel and Zang, 1979).

Figure 4 shows that in one dimension, a singularity of the form $(x-1)^k \log(x-1)$ will produce spectral coefficients that decrease *asymptotically* as $O(1/v^{2k+1})$. A log–log plot like Fig. 4 is a good way to identify such algebraic convergence because the coefficients will approach asymptotically to a straight line with a slope of $-j$ if the coefficients decrease as $O(1/n^j)$.

In two dimensions, the effect of the corner singularities is weakened. Although there is considerable scatter because the coefficients decay in an oscillatory fashion rather than monotonically, the data points for the solution of Poisson's equation can be tightly bounded by a line with a slope of -6, as noted[2] previously in Haidvogel and Zang (1979) and shown here in Fig. 5.

[2] In one dimension, the slope would be -5, but the fact that $u(x, y)$ is singular only at discrete points, not the whole boundary, weakens the effects of the branch points in two dimensions.

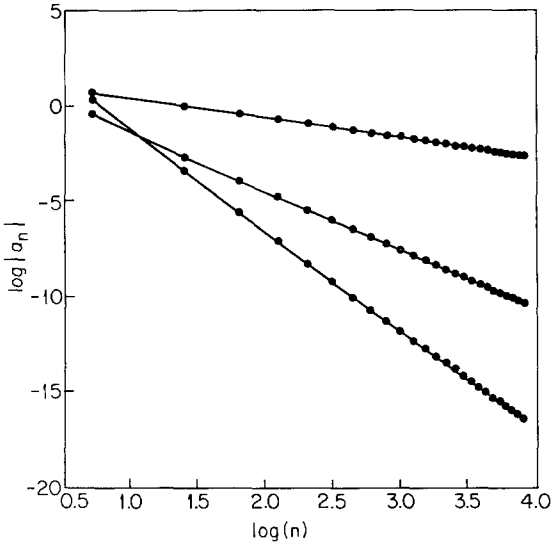

Fig. 4. The logarithm of the absolute value of the Chebyshev coefficients plotted against the logarithm of the degree of the coefficient for three model functions, which have the form $f(x) = (1-x)^k \log(1-x) + (1+x)^k \log(1+x)$ for (top curve) $k = 0$, (middle curve) $k = 1$, and (bottom graph) $k = 2$. The curves approach asymptotically to straight lines with slopes of -1, -3, and -5, respectively, indicating that $|a_n| \sim O(1/v^j)$ for $j = 1$, 3, and 5. The graphs for all three functions would curve downward more and more steeply on this log–log plot (instead of approaching asymptotically to straight lines) were it not for the branch points at $x = \pm 1$.

The graph also shows the pseudospectral coefficients for a moderately nonlinear solution of Bratu's equation. The two clusters of coefficients can be tightly bounded from above by two curves that we will henceforth refer to as the "envelopes" of the Chebyshev coefficients; these are graphed in Fig. 6. Two things are very striking. First, the coefficients for the Bratu $u(x, y)$ lie far above those for the solution of the Poisson equation [except for very large $(m+n)$] even though the forcing for the latter was chosen so that the two would have equally strong corner singularities. The implication is that structure created by the *nonlinear* term of Bratu's equation is much more important in determining the magnitude of the Chebyshev coefficients than are the *corner singularities* unless one is interested in extremely high accuracy. The "envelopes" in Fig. 6 do not intersect until both have logarithms of $O(17)$, that is, until $|a_i| \sim O(10^{-8})$. Although the error of the solution of the differential equation is somewhat larger than the highest coefficients—recall that the coefficients decrease as $O(v^{-6})$, but the error only as $O(v^{-4})$—it is clear that the branch points

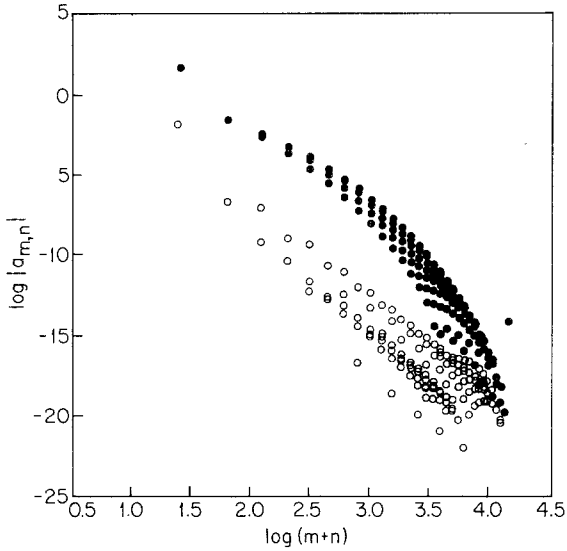

Fig. 5. A plot of the logarithm of the absolute value of the spectral coefficients for the numerical solutions to two problems: (○) Bratu's equation for $\max|u(x, y)| = A = 5$, and (●) Poisson's equation. The x axis is $\log(m+n)$, where the highest degree polynomials in the basis function are $T_m(x)$ and $T_n(y)$. The Poisson equation is $u_{xx} + u_{yy} = -\lambda$, where λ is the Bratu eigenvalue for $A = 5$, so that the strength of the "corner" singularities is the same for both solutions.

may be safely ignored for this case unless one wants more than five digits of accuracy.

In Boyd (1986b) a mapping is described, originally due to F. Stenger, which can be combined with the orthogonal rational function basis described in Boyd (1986c) to solve equations with *exponential* accuracy in spite of weak endpoint or corner singularities. As an experiment, we applied this trick to Bratu's equation, but even for small amplitude (where the corner singularities are of greater relative importance than for $A = 5$), we found that the results with a moderate number of basis functions ($N = 55$) were always inferior to those with no mapping at all.

At first, this seems very puzzling, because the theory in Boyd (1986b) is quite rigorous: for *sufficiently large* N, the mapping will improve accuracy for solutions with corner singularities. The subtlety is that this statement is true only asymptotically. For moderate accuracy—several digits—the most efficient way to solve Bratu's equation using Chebyshev polynomials is to simply *ignore* the corner branch points.

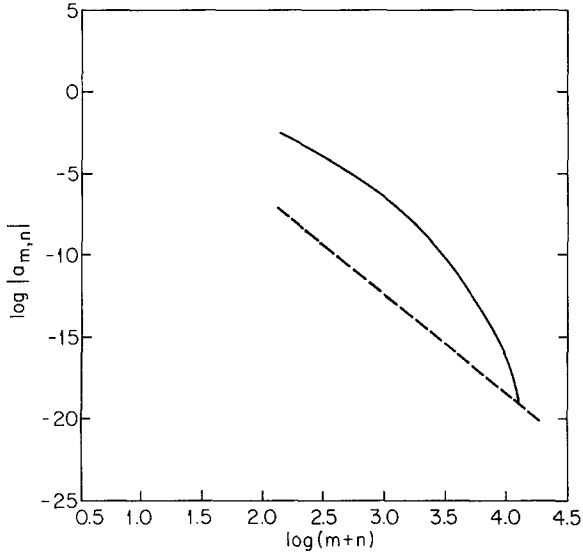

Fig. 6. The curves ("envelopes") that bound the Chebyshev coefficients graphed in Fig. 6. (—) The envelope of the $|a_i|$ for the solution of Bratu's equation; (– –) the envelope for Poisson's equation. The straight-line envelope for the Poisson solution is characteristic of coefficients decaying as $O(1/\nu^6)$. The steep, downward turn of the solid curve is the *exponential* decay with ν, which is typical of a function whose coefficients are dominated by singularities that are not within or on the boundaries.

7. SUMMARY AND CONCLUSIONS

This study has four main conclusions. First, *symmetry* is very important to numerical efficiency. Since the memory for dense matrices scales as $O(N^2)$ and the CPU time for Gaussian elimination as $O(N^3/3)$, the eightfold reduction in the size of the basis via symmetry reduces memory requirements by a factor of 64 and the execution time by about 512. It is striking that one of the three symmetries, the invariance under rotations by integral multiples of 90° in the x–y plane, is a two-dimensional symmetry that does not have a one-dimensional counterpart.

Second, although the pseudospectral method is usually regarded as strictly a numerical algorithm, Sections 3 and 4 show that for Bratu's equation it is a powerful *analytical* tool as well. The approximation

$$\lambda(A) \approx 3.2Ae^{-0.64A} \tag{33}$$

can be derived with paper and pencil in perhaps half an hour, yet it

predicts the maximum value of λ to within about 8.0% and is qualitatively correct for all A.

Finlayson (1972) gives many other examples that fall in this same analytically soluble class. The restriction is that the problem must be simple—a theoretician's problem like the Bratu equation rather than an engineer's task such as calculating the flow around an airliner. Nonetheless, it is still useful to see a two-dimensional nonlinear eigenvalue problem humbled by one-point collocation because it is from such simple examples that we gain both the theoretical understanding and the numerical experience to tackle the very difficult problems that demand a supercomputer.

This in turn justifies the tart words of Birkhoff and Lynch (1984) on the suitability of the Bratu problem as a test of nonlinear eigenvalue solvers: "[it] has been a favorite among mathematicians because of its simplicity, but it is by no means typical. Some idea of the complexity of real heat transport problems can be gained by skimming [the text of] Jacobs." Well, yes: one cannot be too proud of a program that has sucessfully "turned the corner" at the limit point when a back-of-the-envelope approximation like (33) can do the same.[3]

Nonetheless, the simplicity of Bratu's equation does make it a useful tool for testing the *correctness* of a program even if this simplicity makes it inappropriate as a test of robustness. Table III presents the Chebyshev coefficients for $A = 1$ to provide an "exact" solution for such comparison purposes.

This same simplicity also makes Bratu's problem all the more effective for illustrating our third theme: that *corner singularities* are so *weak* that they can be usually be *ignored* in applying spectral methods. Figures 5 and 6 show that the Bratu coefficients a_{mn} for moderate m and n and moderate to strong nonlinearity are an order of magnitude larger than their counterparts for the solution of a Poisson equation that has the same corner singularities but is linear. Replacing Bratu's equation by a more complex problem would merely increase the gap between the coefficients of the solution to the nonlinear equation and those of the Poisson problem.

There *is* a crossover point where the exponential decrease of the Bratu coefficients for moderate m and n is replaced by the slower algebraic decay that is the result of the branch points in the corners of the computational domain. For Poisson's equation, Fig. 5 shows that the corner singularities are important even for coefficients of low degree, and the same is true for Bratu's equation for small amplitude because the nonlinear solution is only a little different from that of the corresponding Poisson problem. For

[3] The author once rederived (33) for a colleague on the back of a paper napkin!

Table III. The Lowest 36 Coefficients for the Solution of Bratu's Equation for $A = 1^a$

m	n	a_{mn}	m	n	a_{mn}
2	2	1	4	2	−0.0051361
4	4	0.0039830	6	2	0.0031676
6	4	0.0002267	6	6	0.0003099
8	2	−0.0001424	8	4	0.0000257
8	6	0.0000710	8	8	0.0000526
10	2	−0.0000236	10	4	−0.0000115
10	6	0.0000130	10	8	0.0000201
10	10	0.0000142	12	2	−0.0000091
12	4	−0.0000052	12	6	0.0000007
12	8	0.0000058	12	10	0.0000067
12	12	0.0000046	14	2	−0.0000028
14	4	−0.0000020	14	6	−0.0000005
14	8	0.0000013	14	10	0.0000023
14	12	0.0000020	14	14	0.0000011
16	2	−0.0000094	16	4	−0.0000086
16	6	−0.0000071	16	8	−0.0000050
16	10	−0.0000027	16	12	−0.0000008
16	14	0.0	16	16	0.0000384

[a] The eigenvalue is $\lambda = 1.62311$, correct to all places shown; the maximum error in the sum of the first 36 coefficients is less than 0.00008. The corresponding basis functions are of the form $\phi_{22} = 0.25\ [1 - T_2(x)][1 - T_2(y)]$, with

$$\phi_{mn} \equiv [1 - T_m(x)][1 - T_n(y)] + \delta_{mn}[1 - T_n(x)][1 - T_m(y)] - p\phi_{22}(x, y)$$

where $\delta_{mn} = 1$ if $m \neq n$ and 0 otherwise and where p is chosen so that the basis function vanishes at the origin, which demands [using (A2)]

$$p = [1 - \cos(m\pi/2)][1 - \cos(n\pi/2)](1 + \delta_{mn})$$

stronger nonlinearity, however, the crossover point occurs only where the expansion, if truncated at that N, would be accurate to several decimal places. Even in the small-amplitude limit where the corner singularities have their largest relative importance, the pseudospectral method still gave answers to five significant figures with less than 80 basis functions.

Our fourth finding is that because of all the symmetries and the negligible impact of the branch points of $u(x, y)$ at the corners, it was possible to solve Bratu's problem to several decimal places on an IBM AT using a dialect of BASIC (True Basic, which is roughly 20 times slower than FORTRAN). Although, as noted by Birkhoff and Lynch in the quote above, Bratu's problem is too simple to be typical, it is reasonable to suppose that if simple nonlinear equations yield to BASIC on a microcomputer, a broad

class of more complicated equations can be tackled through the same Chebyshev pseudospectral/Newton–Kantorovich algorithms on a supercomputer.

Three problems remain for future research. First, is it possible to derive simple analytic approximations to the Bratu solution in the limit $A \to \infty$? Figure 7 shows that as the amplitude increases, $u(x, y)$ becomes more and more sharply peaked about the origin and is radially symmetric except close to the boundaries. The term e^u tends very rapidly to the Dirac δ-function in this same limit and the eigenvalue λ decreases exponentially fast with A.

Second, although Gaussian elimination was quite adequate for the modest N used here, even on a microcomputer, multigrid methods would offer big savings in solving more complicated problems. Chan and Keller (1982) give a good description of multigrid combined with finite-difference methods—one subtlety is that the operator of the linearized equation (25) has both positive and negative eigenvalues for $A > 1.39$ when λ is the parameter and A an unknown—but pseudospectral-cum-multigrid for Bratu's equation remains a problem for the future. Brandt *et al.* (1985) review applications of spectral multigrid to simple linear problems.

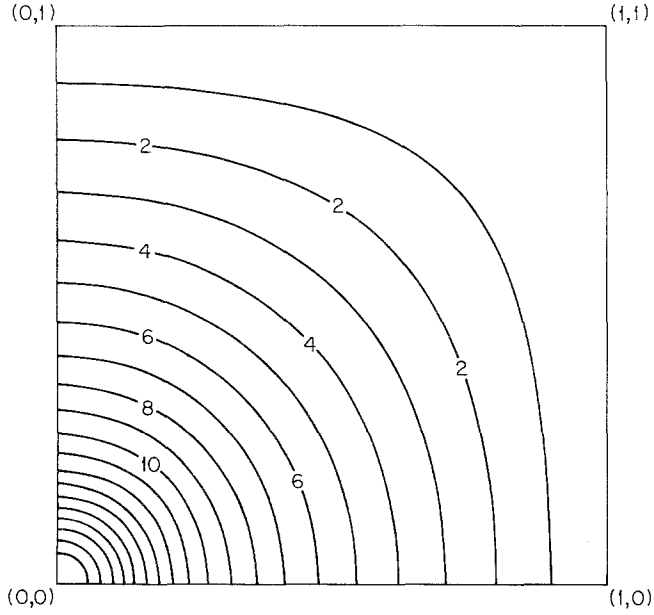

Fig. 7. $u(x, y)$ in the upper right quadrant, $[0, 1] \times [0, 1]$, for $u(0, 0) = 20$. Contours are plotted at unit intervals.

The third issue is: how can pseudospectral methods be extended to deal with stronger singularities such as the $r^{2/3}$ branch point of the L-shaped membrane or the $r^{1/2}$ singularity of the slit square (Birkhoff and Lynch, 1984)? Would the mapping of Boyd (1986b) be useful here?

Nonetheless, in spite of these important problems, we have made progress. The small- and moderate-amplitude analytical approximations have increased our understanding of Bratu's equation; the comparison between the Bratu solution and that of the corresponding Poisson equation has increased our understanding of Chebyshev methods and solutions with weak singularities.

APPENDIX. PROGRAMMING NOTES

One complication in two-dimensional calculations is that the basis functions and interpolation points, which are tensor products of their one-dimensional counterparts, are most naturally described by two indices. To use standard linear algebra software, however, each pair of indices (m, n), where $m = 1,..., v$ and $n = 1,..., m$, must be condensed into a single index $i(m, n)$, where $i = 1,..., N$. The most convenient way to do this is through a preprocessing step that is a double DO or FOR loop in m and n. Whenever the pair of numbers (m, n) passes the appropriate symmetry test ($n \leqslant m$ in this case, although much more complicated conditions are possible in other problems), the "condensed index" i is incremented by 1 and the pair (m, n) is stored in arrays:

$$i \to i + 1, \qquad i = 1,..., N$$

$$ma(i+1) = m, \qquad na(i+1) = n \tag{A1}$$

Whenever one needs to evaluate a basis function, the indices m and n for the ith basis function are retrieved from the N-element arrays $ma(i)$ and $na(i)$. The interpolation points are similarly stored as arrays $xa(i)$ and $ya(i)$.

The second programming issue is that of evaluating the Chebyshev polynomials and the basis functions. The traditional method, described in Gottlieb and Orszag (1977), is to evaluate the Chebyshev polynomials by a three-term recurrence, which costs $O(1)$ operations per polynomial per grid point if all the polynomials at a given grid point are evaluated at once. Similar recurrences (Boyd, 1978) can be evaluated to compute the derivatives.

Here, the programs employed an alternative based on the identity

$$T_n(x) \equiv \cos(nt) \tag{A2}$$

where

$$t = \arccos(x) \tag{A3}$$

The needed derivatives with respect to x are simply linear combinations of the derivatives of $\cos(nt)$ with respect to t. For example,

$$d^2T_n/dx^2 = [(\sin t)(-n^2 \cos nt) - (\cos t)(-n \sin nt)]/\sin^3 t \tag{A4}$$

Since the trigonometric functions and their inverses are built into most compilers—and computed in hardware even on machines as humble as the IBM PC—this alternative is accurate and efficient.

Running time is decreased by storing the values of the basis functions and their derivatives at the grid points as two-dimensional arrays. Unfortunately, this limits the size of the largest basis set that will fit in memory, so the program was rewritten to recompute the basis functions on demand. All N functions are evaluated in a single subroutine for a given x and y. Nonetheless, even with careful optimization, the cost of recomputing the basis functions was as expensive as the UL factorization until $N > 100$. This is true in spite of the fact that basis function evaluations are $O(N^2)$ and the UL factorization is $O(N^3/3)$—a much larger cost in the limit $N \to \infty$.

The empirical result that forming the matrix equation (28) was as expensive as solving it for moderate N reiterates the theme of Section 6: asymptotic estimates must be taken with a grain of salt because often N must be enormous before these estimates are even qualitatively correct. The corner singularities dominate the asymptotic magnitude of the Chebyshev coefficients and yet are irrelevant if N is small enough to give a "mere" five digits of accuracy. Similarly, whether the basis functions are evaluated once or many times is asymptotically unimportant, but for practical values of N, storing the basis function values will drastically reduce CPU time.

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