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All roots spectral methods: Constraints, floating point arithmetic and root exclusion

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ABSTRACT

The nonlinear two-point boundary value problem (TPBVP for short)

$$u_{xx} + u^3 = 0, u(0) = u(1) = 0,$$

offers several insights into spectral methods. First, it has been proved *a priori* that $\int_0^1 u(x)dx = \pi/\sqrt{2}$. By building this constraint into the spectral approximation, the accuracy of $N + 1$ degrees of freedom is achieved from the work of solving a system with only N degrees of freedom. When N is small, generic polynomial system solvers, such as those in the computer algebra system Maple, can find all roots of the polynomial system, such as a spectral discretization of the TPBVP. Our second point is that floating point arithmetic in lieu of exact arithmetic can double the largest practical value of N. (Rational numbers with a huge number of digits are avoided, and eliminating M symbols like $\sqrt{2}$ and π reduces $N+M$-variate polynomials to polynomials in just the N unknowns.) Third, a disadvantage of an "all roots" approach is that the polynomial solver generates many roots – (3^N-1) for our example – which are genuine solutions to the N-term discretization but spurious in the sense that they are not close to the spectral coefficients of a true solution to the TPBVP. We show here that a good tool for "root-exclusion" is calculating $\rho \equiv \sqrt{\sum_{n=1}^{N} b_n^2}$; spurious roots have ρ larger than that for the physical solution by at least an order of magnitude. The ρ-criterion is suggestive rather than infallible, but root exclusion is very hard, and the best approach is to apply multiple tools with complementary failings.

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1. Introduction

The two-point boundary-value problem

$$u_{xx} + u^3 = 0, \qquad u(0) = u(1) = 0 \tag{1}$$

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has the exact solution

$$u = 2\mathcal{K}\text{cn}(2\mathcal{K}(x - 1/2), 1/\sqrt{2}), \qquad \mathcal{K} = 1.85407 \tag{2}$$

where "cn" is the usual Jacobian elliptic function and $\mathcal{K} = K(1/\sqrt{2})$ is the complete elliptic integral for an elliptic modulus $k = 1/\sqrt{2}$. Boyd showed that the problem is "cryptoperiodic" in the sense the most efficient spectral basis is a Fourier basis [1] because the elliptic function is periodic. Here, we apply a polynomial basis partly for comparison and partly and more importantly because polynomial approximations are more widely used than the Fourier basis.

Although difficult problems require N very large where N is the number of degrees of freedom, spectral methods are so powerful that they are often accurate even for very small N. This makes it possible to bypass Newton's iteration and its ilk by applying a polynomial system solver to find all its zeros. This system of N equations in N unknowns is the spectral discretization of the TPBVP and the unknowns are the coefficients of the Chebyshev polynomial approximation [1,2].

2. Imposing an integral constraint

N can be minimized by incorporating symmetry and boundary conditions into the form of the approximation. Here $u(x)$ is symmetric with respect to reflection about the midpoint of the interval [1]; this symmetry can be imposed by including only basis functions with the same symmetry, that is, only even degree (shifted) Chebyshev polynomials, yielding

$$u_N(x) = x(1 - x) \left\{ b_0 + \sum_{n=1}^{N} b_n T_{2n}(2x - 1) \right\}. \tag{3}$$

Independent of the coefficients b_n, $u_N(0) = u_N(1) = 0$ and $u_N(1 - x) = u_N(x)$.

Gheorghiu and Trif [3] observed that

$$\int_0^1 u(x)dx = \pi/\sqrt{2}. \tag{4}$$

This can be used to express b_0 in terms of the other b_n. We assume that the two boundary conditions will be incorporated into the algorithm also. Thus, although the approximation contains only N degrees of freedom, it is a polynomial of degree $(N + 2)$ and thus a polynomial with $(N + 3)$ coefficients.

Table 1 shows that for this smooth problem, albeit a cubically nonlinear problem, the four degree of freedom approximation has a maximum pointwise error which is only 1/14,600 of the maximum of $u(x)$. The complete Maple listing is given in Table 2.

The theory and practice of low degree polynomial spectral methods are described in Chapter 20 of [4], Chapter 2 of [5], Chapters 1 through 6 of [6], the review [7] and [1,7,8].

3. The downside of exact arithmetic

In our Maple 15 system running in Windows 7, the largest feasible number of degrees of freedom was limited by system crashes to $N_{feasible} = 2$ when exact arithmetic was used as far as possible in the computation. $N_{feasible}$ was *doubled* by altering a single line:

$$r[m] -> evalf(r[m]) \tag{5}$$

where $r[m]$ is the mth equation of Galerkin system and where "evalf" is the Maple command to force replacement of symbols like $\sqrt{2}$, π and $BesselJ(0)$ by their floating equivalents. Why does "evalf" make such a difference?

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