Adaptive Methods for Piecewise Polynomial Collocation for Ordinary Differential Equations

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April 24, 2003

1 Introduction

This paper first gives a brief survey of background work on collocation methods relevant to the main part of the paper. This main part concerns adaptive methods for piecewise polynomial collocation, where various criteria are compared. Use of both interval subdivision, where a current subdivision has one sub-interval halved, and interval redistribution, where a completely new subdivision is chosen, are considered. Interval selection aims to obtain a set of intervals where the criterion is equidistributed, that is the criterion has the same value in each sub-interval. The emphasis here is on the choice of criterion rather than the production of a complete algorithm, which it is hoped will be considered in a later paper. The equidistribution strategy seems natural and is effective at least when the solution is reasonably accurate. However, when the accuracy is poor, it is shown by example that more than one subdivision may produce equidistribution, and the optimal choice of subdivision may not correspond to equidistribution.

2 Background

In this paper only linear ordinary differential boundary value problems of the form of either a single higher order differential equation

$$x^{(m)}(t) + \sum_{j=0}^{m-1} p_j(t)x^{(j)}(t) = y(t) \tag{1}$$

or a system of first order differential equations

$$\mathbf{x}' + \mathbf{A}(t)\mathbf{x} = \mathbf{y}(t) \tag{2}$$

with suitable boundary conditions are considered. However, all illustrative results concern higher order equations. Non-linear equations can often be treated by iteration of a sequence of linear problems, but that aspect will not be considered here.

Both forms of equation can be represented in operator form:

$$(D^m - T)x = y. \tag{3}$$

Given an approximate solution x_n, where n indicates the number of unknowns in the approximate solution, the residual r_n can be definined by:

$$r_n = (D^m - T)x_n - y. \tag{4}$$

The global polynomial collocation method sets $r_n = 0$ at some set of collocation points

$$\xi_k, \quad k = 1 \dots q,$$

so that the number of equations, including boundary conditions is equal to the number of parameters in x_n. For piecewise polynomial collocation similarly distributed points are used in each sub-interval. If the range (a, b) is subdivided using the break-points

$$a = t_0 < t_1 < \dots < t_p = b$$

the points used in interval $[t_j, t_{j+1}]$ will be given by

$$x_{jk} = 0.5((t_{j+1} - t_j)\xi_k + (t_{j+1} + t_j)), \quad k = 1 \dots q, \tag{5}$$

with the ξ_k in $(-1, 1)$. Usually the same number of points is used in each sub-interval. The number of points is chosen so that along with the boundary and join conditions the number of equations is the same as the number of unknowns.

The idea of collocation is rather obvious and has a long history. However, the location of the points is important. Lanczos [7] suggested using Chebyshev polynomial zeros for global polynomial collocation. With q collocation points the residual r_n will have a factor

$$w(t) = \prod_{k=1}^{q} (t - \xi_k)$$

and $\|w\|_\infty$ is minimised with this choice of Chebyshev zeros. For piecewise polynomial collocation the residual will have a similar factor in each subinterval.

Super-convergence for piecewise polynomial collocation (as the number of intervals increases with fixed degree in each interval) using Gauss points is shown by de Boor and Swartz [5]. Because of this result this choice of points, rather than Chebyshev zeros, is used in all the illustrations.

The error is related to the residual by

$$e_n = (D^m - T)^{-1} r_n \tag{6}$$

so minimising the residual is a reasonable aim though not necessarily the best policy.

The approximate solution can be represented in a number of different ways. The calculations for the illustrations used a local Chebyshev series in each sub-interval. For this purpose each sub-interval is mapped onto the interval $(-1, 1)$ in a similar way to equation (5).

The collocation equations can be written in operator form as

$$\phi_n (D^m - T) x_n = \phi_n y$$

where ϕ_n is the (piecewise) polynomial interpolation projection operator associated with the collocation points.

If $\phi_n D^m x_n = D^m x_n$ then the eqution becomes

$$(D^m - \phi_n T)x_n = \phi_n y. \tag{7}$$

Results on computable error bounds and estimates developed from this equation are considerd by Ahmed and Wright [1] and Wright[11]. Many of these are dependent on finding a bound or estimate for

$$\|(D^m - T)^{-1}\|.$$

In Ahmed and Wright [2] it is shown that there is a computable matrix Q_n such that

$$\|Q_n\| \to \|(D^m - T)^{-1}\|.$$

Calculation of Q_n involves the inverse of the collocation matrix and so is relatively expensive to evaluate, but can be used to give estimates of bounds on error using the inequality

$$\|e_n\| \leq \|(D_m - T)^{-1}\| \|r_n\|$$

derived from (6).

A cheaper alternative is to use the identity

$$(D^m - T)^{-1} = (D^m)^{-1} + (D^m - T)^{-1}K$$

where $K = TD^{-1}$, which suggests replacing the $(D^m - T)^{-1}$ on the right hand side by the approximate operator

$$(D^m - \phi_n T)^{-1}\phi_n$$

as in the original approximation to the differential equation (7), giving error estimate:

$$e_n \approx e_n^* = (D^m)^{-1} r_n + (D^m - \phi_n T)^{-1}\phi_n K r_n. \tag{8}$$

This produces the error estimate which is a function of t. It involves integration of r_n, some manipulation to find Kr_n and a second linear equation solution with the same matrix as the original solution.

Note that r_n needs to be estimated somehow, for example by evaluation at a mesh of points over the interval followed by interpolation. A particularly convenient choice is to use the appropriate Chebyshev polynomial extrema using one more point than used for the collocation solution in each sub-interval (with approprate range transformation). The aim of this is that these points are likely to give values near the extrema of the residual, particularly if Chebyshev zeros are used, but also for Gauss points as the distribution is fairly similar.

3 Adaptive Methods - Piecewise Polynomial Collocation

For developing an adaptive scheme for piecewise polynomial collocation there are rather a lot of choices. In particular decisions need to be made about:

- Initial Distribution
- Criterion
- Subdivision or Redistribution
- Single or Multiple Incrementation

There are many possibilities for criteria such as

- Derivative size
- Maximum residual
- Error estimate
- de Boor [4] criterion
- Maximum residual * interval size
- Last Chebyshev coefficient.

Given some criterion it seems quite natural to attempt to choose a set of sub-intervals so that the criterion is roughly equal in every sub-interval, either by subdividing the sub-interval (or intervals) which have the largest criterion values: interval subdivision, or by choosing a completely new set of subintervals: interval redistribution.

These issues are discussed in de Boor [4], Russell and Christiansen [10], and in an abstract setting by Rheinboldt [9], and [8]. Further discussion and empirical results for interval subdivision are given in Wright, Ahmed and Seleman [12].

Subdivision algorithms are straightforward to implement as they only require finding the interval(s) with the largest criterion values. Redistribution on the other hand needs an estimate of how the criterion will vary as interval size changes. This is based on the asymptotic behaviour of the criterion with respect to interval size. Even though this is not strictly valid in the early stages of the calculations, there does not seem to be any obvious alternative.

The new break-points are found by an inverse interpolation process described by de Boor [4]. This uses a piecewise linear function with slopes in each sub-interval based on $c^{1/p}$ where c is the criterion value and h^p is the asymptotic order of the criterion in terms of the interval size h.

In this paper we only consider single incrementation that is only increasing the number of sub-intervals by one at each stage. The possibilities for multiple incrementation are very many and are currently being investigated.

4 Motivation for criterion choice

It is clear that the choice of criterion should be such that the new set of sub-intervals produce as small errors as possible, while not being unreasonably expensive to implement. There may well be a conflict between these considerations.

Perhaps the most intuitively simple criterion is to use some norm of a derivative of the approximate solution in each sub-interval. However, this does not have a clear theoretical justification, except for the highest order derivative which is related to the local error. The choice of highest order derivative is also related to the highest degree Chebyshev coefficient of the approximate solution. This is essentially a rescaling with the (constant) highest derivative being given by Cc_n/h^n where h is the sub-interval size, n the highest degree, c_n the last coefficient and C a constant independent of h. It is of course possible that the coefficient c_n may be accidentally small (for example in the case of symmetric or anti-symmetric functions) and this might cause problems. With the solution represented as local Chebyshev series then essentially no extra work is required to produce the criterion.

The use of an estimate of the maximum residual was suggested by Carey and Humphrey [3]. The residual can easily be evaluated at any individual point and taking into account that it is zero at the collocation points an estimate of the maximum residual $\|r_j\|$ in each sub-interval is not very difficult. As the residual is related to the error by (6) even though the residual is oscillatory this seems a reasonable criterion. However, empirical results presented below give rather poor results. As the error equation (6) can be re-written as an integral of the form

$$e(t) = \int_a^b G(t,s)r(s)ds \tag{9}$$

$$= \sum_{j=1}^{p} \int_{t_j}^{t_j+1} G(t,s)r(s)ds$$

where $G(t,s)$ is the Green's function associated with the differential operator. The right hand side is less than

$$\sum_{j=1}^{p} h_j \|G(t,s)\|_s \|r_j\|$$

where $h_j = t_{j+1} - t_j$. Athough this is a rough bound it indicates the dependence on h_j, and that $h_j\|r_j\|$ would be a more appropriate criterion than $\|r_j\|$ itself.

The criterion given by de Boor [4] uses a local error estimate based on the changes in the highest derivative in adjacent intervals, and this has been widely used.

At first sight the most appropriate criterion to use would seem to be an estimate of the maximum global error in each interval, though this might be expensive to evaluate. The estimate (8) can be used in this way. This sometimes gives very good results but in other cases can be completely unsatisfactory as will be shown in the examples below.

5 Illustrative Examples

Results for a number of simple differentiual equations with boundary or interior layers are given. All the examples use Gauss point collocation.

The criteria used are:

- DB: de Boor
- R: Maximum Residual - estimated by evaluation at $q+1$ Chebyshev extrema in each sub-interval
- HR: R mutiplied by sub-interval size
- EST: The maximum absolute estimate of the global error using (8) in each sub-interval.
- CC: The absolute value of the last Chebyshev coefficient in each sub-interval.

The test differential equations have been chosen with known exact or asymptotic solutions so that the errors can easily be compared. The examples used are:

Problem A:

$$y'' - \mu y' - (1+\mu)y = 0,$$

$$y(0) = 1 + \exp(-(1+\mu)), \;\; y(1) = 1 + \exp(-1)$$
$$y = \exp((1+\mu)(t-1)) + \exp(-t)$$

Boundary layer at upper end, $(\mu >> 0)$

Problem B:

$$y'' + \mu y' = -\pi^2 \cos(\pi t) - \mu \pi t \sin(\pi t)$$

$$y(-1) = -2, \;\; y(1) = 0$$
$$y = \cos(\pi t) + \mathrm{erf}(wt)/\mathrm{erf}(w)$$

where $w = \sqrt{(\mu/2)}$

Interior layer at $t = 0$, $(\mu >> 0)$

Problem C:

$$y'' - \mu(2 - t^2)y = -\mu,$$

$$y(-1) = y(1) = 0$$

$$y \to 1/(2 - t^2) - \exp(-\sqrt{\mu}(1 + t)) - \exp(-\sqrt{\mu}(1 - t)), \text{ as } \mu \to \infty$$

Boundary layers at both ends, $(\mu >> 0)$

Problem D:

$$y^{iv} - (\lambda + \mu)y''' + (\lambda\mu - 1)y'' + (\lambda + \mu)y' - \lambda\mu y = 0$$

$$y(0) = e^{-\lambda} + e^{-\mu} + 2$$

$$y'(0) = \lambda e^{-\lambda} + \mu e^{-\mu}$$

$$y(1) = 2 + e + e^{-1}$$

$$y'(1) = \lambda + \mu + e + e^{-1}$$

$$y = e^{\lambda(t-1)} + e^{\mu(t-1)} + e^t + e^{-t}$$

Boundary layer at ends, $(\lambda >> 0, \mu << 0)$

Problem E:

$$y^{iv} - (\lambda + \mu)y''' + (\lambda\mu + 1)y'' - (\lambda + \mu)y' + \lambda\mu y = 0$$

$$y(0) = 1 + e^{-\lambda}$$

$$y'(0) = \lambda e^{-\lambda} + \mu + 1$$

$$y(1) = 1 + e^{\mu} + \sin(1)$$

$$y'(1) = \lambda + \mu e^{\mu} + \cos(1)$$

$$y = e^{\lambda(t-1)} + e^{\mu t} + \sin(t)$$

Boundary layer at ends, $(\lambda >> 0, \mu << 0)$

The results show graphs of error estimates and errors (where available) for the different criteria and equations. The errors are estimated by evaluating the difference between the true solution and approximation over a fine mesh over the whole interval. The error estimates are based on the error estimation equation (8).

Naturally only a small selection of examples can be illustrated, but the ones chosen do illustrate the problems with some of the criteria and give an indication of their relative merit.

The following notation is used in the graphs:

******** DB: DeBoor

++++++++ R: Residual

xxxxxxxx hR: Residual* Interval Size

oooooooo Est: Error Estimate.

-.-.-.-. CC: Last Chebyshev Coefficient

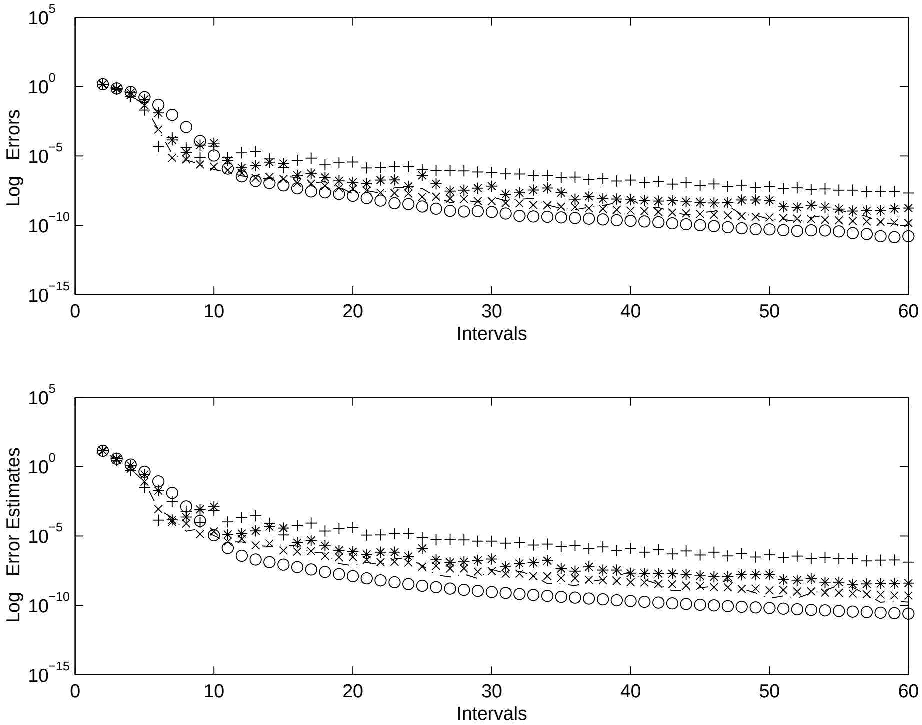

Figure 1: Redistribution: Problem A, $\mu = 100$, 4 Points

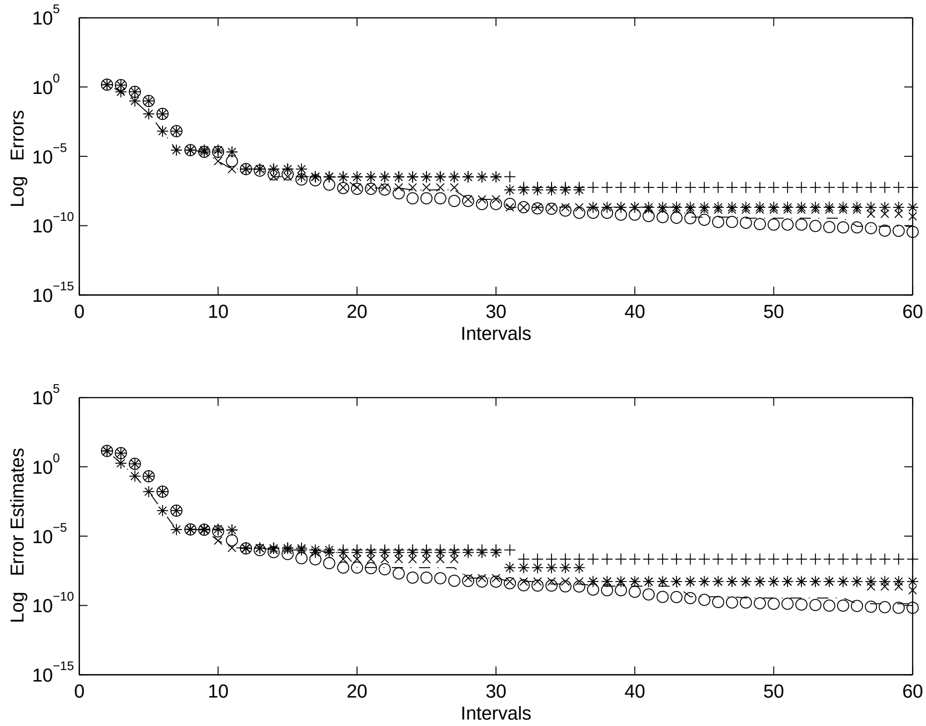

Figure 2: Subdivision: Problem A, $\mu = 100$, 4 Points

Problem A has a relatively mild boundary layer and Figures 1 and 2 show that all criteria behave reasonably well, though R is clearly the worst and the EST the best. Figure 2 shows also a phenomenon common with interval subdivision where the error and error estimate can remain the same for many iterations, while redistribution gives smoother convergence.

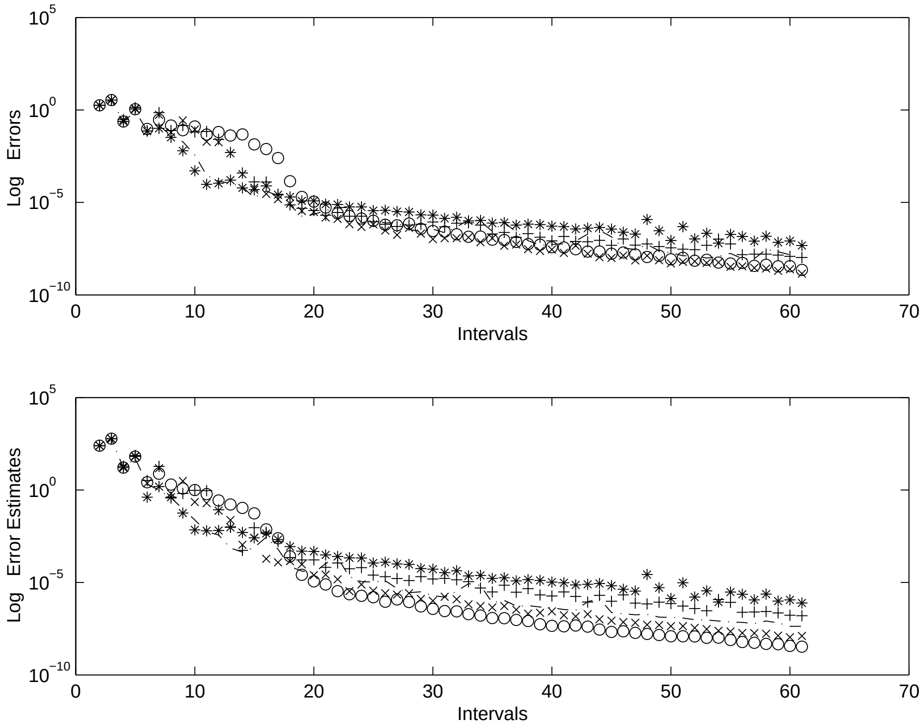

Figure 3: Redistribution: Problem B, $\mu = 1000$, 4 Points

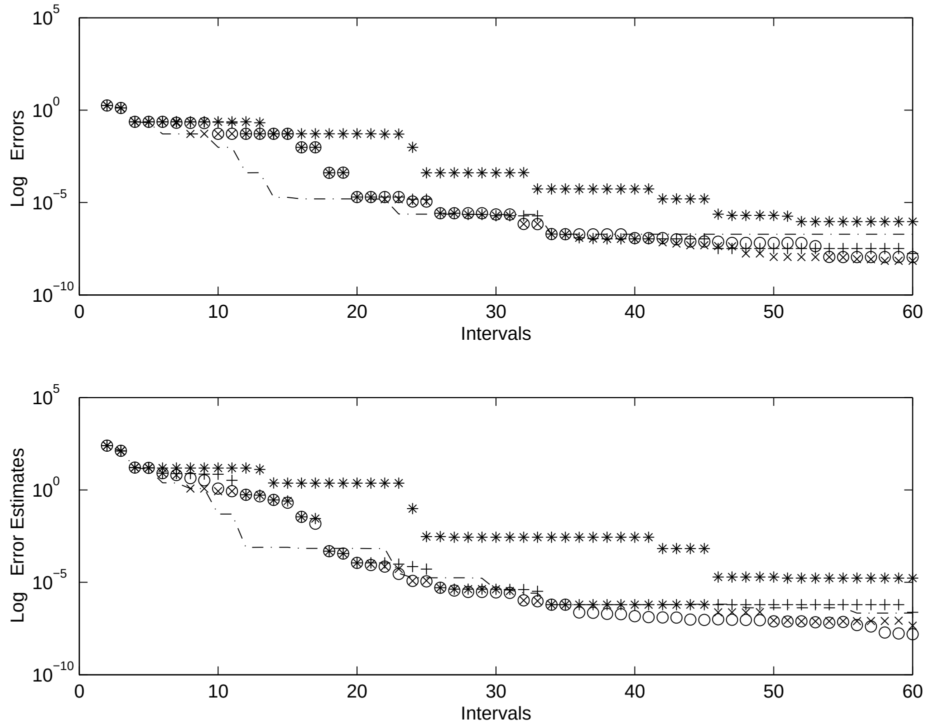

Figure 4: Subdivision: Problem B, $\mu = 1000$, 4 Points

Figures 3 and 4 for problem B which has an interior layer show rather similar behaviour to problem A, though here the DB criterion gives the poorest results and the HR and EST give the best. Note that there is unfortunate confusion in Figure 4 as the symbols `+` and `x` combine to look the same as `*`. On account of the rather unsatisfactory behaviour of the interval sub-division process, the remaining graphs all show just results for redistribution.

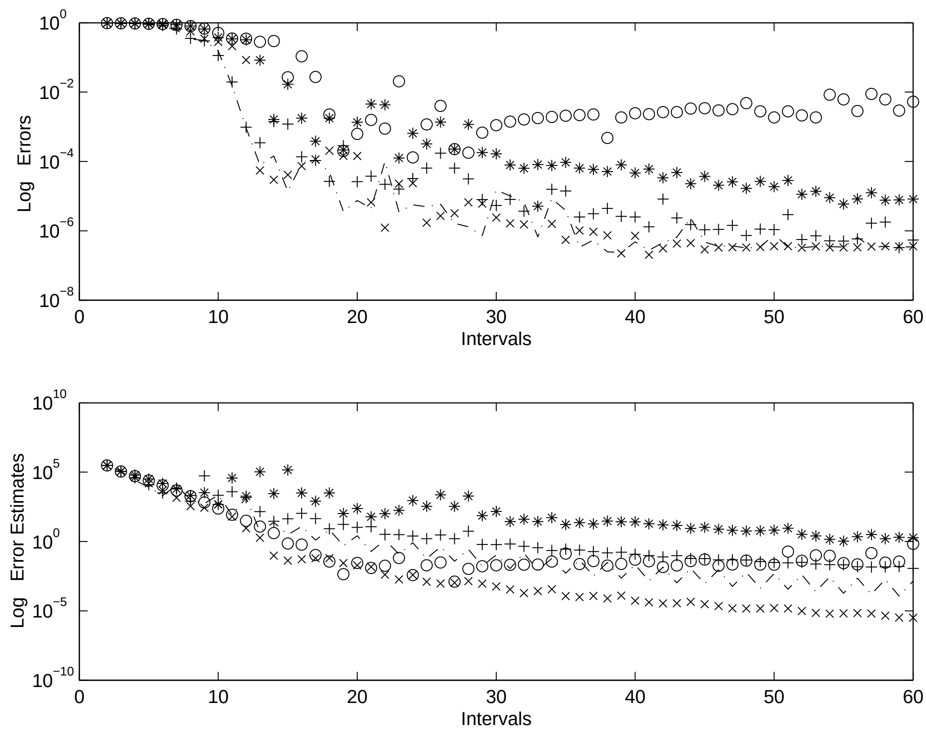

Figure 5: Subdivision: Problem C, $\mu = 1e8$, 4 Points

For problem C which has boundary layers at both ends of the range, figure 5 shows that the EST criterion can be completely unsatisfactory. It also shows rather poor results for DB, while HR seems to give the best results. Though subdivision results for this problem are not illustrated, the DB and EST criteria appear to give no improvement after the initial phase. The errors for HR and CC in this case are limited by the accuracy of the asymptotic solution used for comparison.

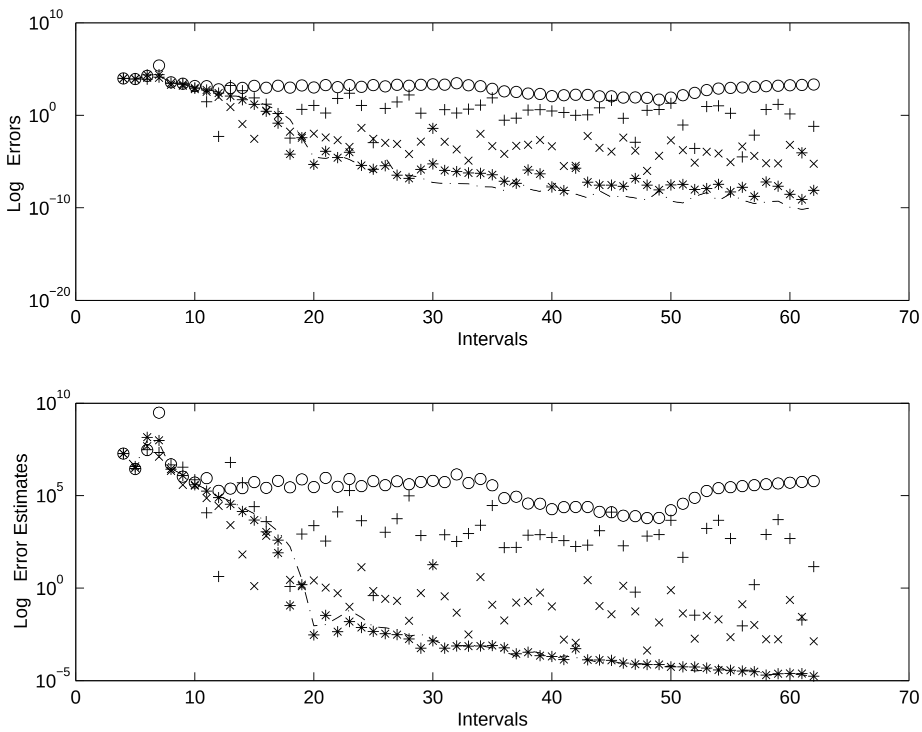

Figure 6: Subdivision: Problem D, $\lambda = 1000$, $\mu = -0.5$, 3 Points

Figure 6 illustrates the 4th order problem D which has a boundary layer at the upper end of the range. Here EST and R give unsatisfactory results, while DB and CC are best.

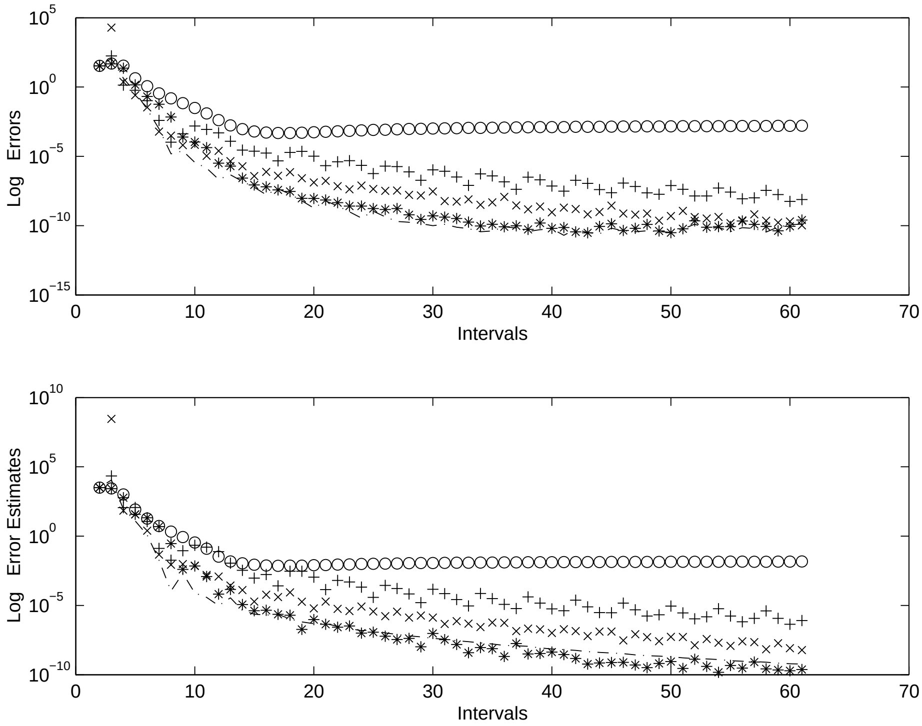

Figure 7: Redistribution: Problem E, $\lambda = 200, \mu = -50$, 4 Points

Problem E illustrated in Figure 7 has boundary layers at both ends of the range with the left-hand layer more mild than the right-hand layer. The results are similar to problem D, but the layers here are less severe.

These illustrations show erratic behaviour in the initial stages where the accuracy is low, but in later stages at least some of the calculations proceed in a very smooth manner.

As the basis of a generally applicable method it is most important that the criterion should give reliable results for a wide range of problems rather than produce very good results occasionally. This excludes the use of the error estimate as a criterion, in spite of its good performance on problems A and B, and its overall quality as an error estimate. The situation can perhaps be understood by considering the Green's function in the relation between residual and error (9). In many cases the Green's function is dominated by the diagonal $t = s$ but this is not always true particularly for (mildly) ill-conditioned problems. In these cases the largest error may not occur in the same sub-interval as the residual which most contributes to it so the interval reduction does not occur in the most appropriate place. This is in spite of the result given by Russell and Christiansen [10] that the global error is asymptotically dominated by local terms when Gauss point collocation is used.

The behaviour of the residual criterion R is generally rather poor and even unsatisfactory for problems D and E. The modification to give the HR criterion produces a very significant improvement, and performs reliably in all cases, though not as well as DB and CC on the problems D and E.

The de Boor DB criterion generally performs well, though for problem C it is poor bordering on unsatisfactory. It seems particularly good on the fourth order problems D and E.

The last Chebyshev coefficient CC criterion performs remarkably well using redistribution considering that it is expected to be unsatisfactory in cases where the last coefficient is 'accidentally' small. This behaviour with redistribution can be understood by considering the inverse interpolation process involved in the redistribution algorithm, where the new interval size will depend on intervals adjacent to the one with a small criterion value as well as that interval itself. With interval subdivision on the other hand even though the results illustrated in figures 2 and 4 are reasonable, an interval with a small criterion value can remain unchanged throughout, and so produce misleading and unsatisfactory results.

The results also illustrate that even though the error estimate is not reliable as a criterion for subdivision it is reliable as an estimate of the error once the calculations have settled down, and is almost always larger than the actual error.

Similar results also apply for systems of first order ordinary differential equations and these are discussed in detail in Hermansyah PhD thesis [6], which also considers prediction of number of intervals needed and initial selection of intervals.

There is no difficulty in increasing the number of intervals by more than one, though in the early stage of the process the prediction may be much too large, so any algorithm needs to take this into account. Various heuristic strategies are possible to deal with this and are currently being investigated.

6 Optimal interval sizes

For 2 sub-intervals equi-distributing points can always be found by a bisection type process.

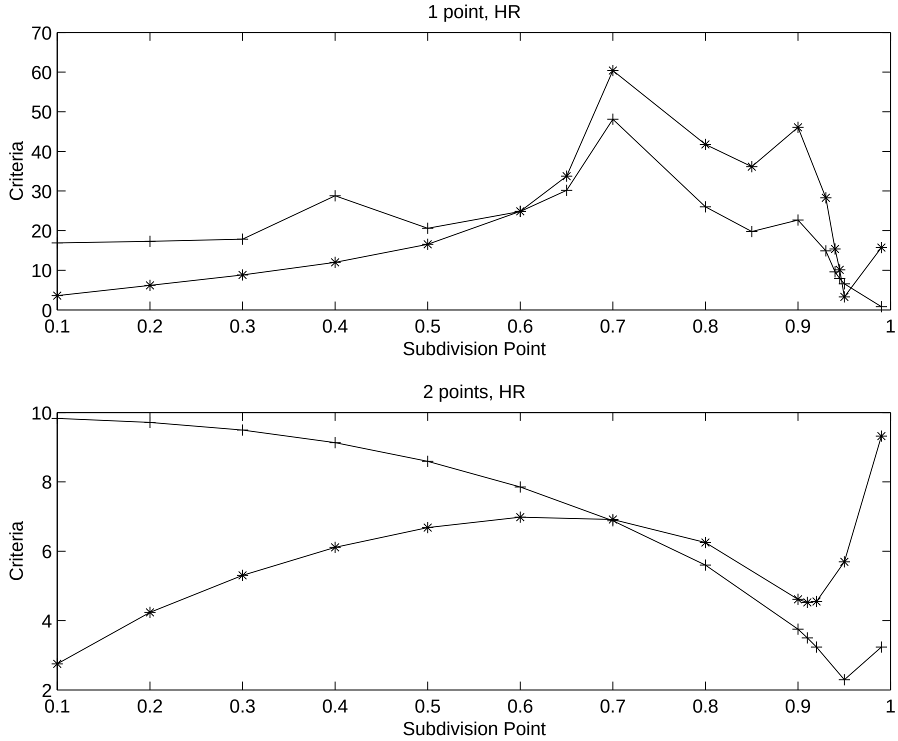

Figure 8: Criteria vs Division Point: 2 Intervals, Problem A, $\mu = 40$.

For the HR criterion the graphs in Figure 8 show that for 2 sub-intervals when there is one collocation point there are three points where the criteria are equal, illustrating that equidistribution may not be unique and with only one optimal. The graph for 2 collocation points shows that the smallest criteria values may not occur when the criteria are equal. Similar behaviour occurs with other criteria except DB where the formulae are special for 2 sub-intervals.

Iterating the redistribution process with a fixed number of sub-intervals sometimes converges to an optimal distribution of intervals, but even when the iteration converges it may converge to a non-optimal equidistributing subdivision.

7 Conclusions

The results indicate clearly that interval redistribution is a more reliable process than interval subdivision. Even though there are potential economies in the subdivision process this does not make up for its unreliability.

The examples strongly suggest that a criterion based on a global error estimate will not be satisfactory for all problems. They also suggest that the maximum residual is not a reliable criterion. On the other hand they do suggest that both the last Chebyshev coefficient CC and HR criteria are competitive with the de Boor criterion DB and may be preferable. As the CC criterion gives good results and requires little calculation, but still has the possibility of giving an interval which is too large, an algorithm using more than one criterion may be worth investigating. The CC and HR criteria would fit well together for this as they are completely independent.

The non-uniqueness of equi-distribution suggests a need for caution in its use. However, this does not appear to cause any problems once the solution is reasonably accurate.

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