Numerical solution of unstable initial value problems by invariant imbedding*

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This paper shows how a generalised Ricatti transformation, which grew out of the study of invariant imbedding, may be used to convert certain unstable linear second order initial value problems into equivalent initial value problems which are often quite stable.

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1. Introduction

The method of invariant imbedding was originally developed on a 'particle' counting basis for investigating the reflection and transmission functions of radiative transfer and neutron transport (Wing, 1962). Later it was recognised that the imbedding involved a perturbation on the 'size' of the system. This led to more of a 'mechanistic' approach to the procedure, and allowed the conversion of two-point boundary problems into initial value problems independent of the physical origin of the differential equations under consideration (Bellman and Kalaba, 1961). In the process of numerical experimentation, it was observed that the Ricatti equations of invariant imbedding are generally quite stable. Several papers have appeared which use this fact to convert boundary value problems into stable initial value problems (Bellman, Kagiwada and Kalaba, 1966 and 1967; Scott, 1969). In this paper we will show how a generalised Ricatti transformation, which grew out of the study of invariant imbedding, may be used to convert certain unstable linear second order initial value problems into equivalent initial value problems which are often quite stable. In addition, we will discuss the applicability of backward integration to certain types of unstable problems.

There are several different cases in which initial value methods are either directly applicable, undesirable, or must be slightly modified. The direct forward integration is stable when the growth of the wanted solution is the same or greater than the growth of the dominant complementary solution. If it happens that both solutions of the homogeneous equation rise faster than or decrease slower than the true solution, then backward integration may be more appropriate, since both complementary solutions then decrease faster or rise slower than the solution which is sought and, hence, usually cause no trouble. The case that usually causes the most trouble is where the solution growth is between the complementary solutions. Here neither forward nor backward integration is stable, and very special techniques may be required.

Other excellent approaches for solving unstable initial value problems which use boundary value techniques are discussed in Fox and Mitchell (1957) and Greenspan (1967). Although the problems of stability are often eliminated in the boundary value techniques, the questions of existence and uniqueness may be troublesome. For example, the initial value problem

$$y'' + \pi^2 y = 0, \tag{1.1}$$

$$y(0) = 0, \tag{1.2}$$

$$y'(0) = 1, \tag{1.3}$$

has a unique solution over any finite interval, while the boundary value problems defined by (1.1), (1.2) and

$$y(1) = 0, \tag{1.4}$$

and (1.1), (1.2) and

$$y(1) = 1, \tag{1.5}$$

have, respectively, *infinitely* many solutions and *no* solution. Thus it is clear that, when using boundary value techniques, care must be exercised.

2. Formal results

We shall first consider two first-order linear equations of the form

$$u'(z) = a(z)u(z) + b(z)v(z) + e(z), \tag{2.1}$$

$$-v'(z) = c(z)u(z) + d(z)v(z) + f(z), \tag{2.2}$$

with the initial conditions

$$u(0) = \alpha,\ v(0) = \beta, \tag{2.3}$$

where, for simplicity, α and β are real constants and the functions a, b, c, d, e, and f are continuous and real valued on $(0, \infty)$.

From the method of invariant imbedding, we have the relations

$$u(z) = R_1(z)v(z) + \alpha R_2(z) + R_3(z), \tag{2.4}$$

$$\beta = Q_1(z)v(z) + \alpha Q_2(z) + Q_3(z). \tag{2.5}$$

The reader is referred to Nelson and Scott (1969) for a physical motivation of the above relations. We shall now derive differential equations for the functions $R_1(z)$, $R_2(z)$, $R_3(z)$, $Q_1(z)$, $Q_2(z)$, and $Q_3(z)$. If we differentiate in (2.4) and use (2.1) and (2.2), we obtain

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$$v(z)\{R_1'(z) - b(z) - a(z)R_1(z) - d(z)R_1(z) - c(z)R_1^2(z)\} + \alpha\{R_2'(z) - c(z)R_1(z)R_2(z) - a(z)R_2(z)\} + \{R_3'(z) - c(z)R_1(z)R_3(z) - R_1(z)f(z) - e(z) - a(z)R_3(z)\} = 0. \quad (2.6)$$

Equation (2.4) will be satisfied if each term in the braces is set equal to zero. That is,

$$R_1'(z) = b(z) + [a(z) + d(z)]R_1(z) + c(z)R_1^2(z), \quad (2.7)$$

$$R_2'(z) = [a(z) + c(z)R_1(z)]R_2(z), \quad (2.8)$$

$$R_3'(z) = [a(z) + c(z)R_1(z)]R_3(z) + f(z)R_1(z) + e(z). \quad (2.9)$$

Suitable initial conditions, suggested by (2.3) and (2.4), are

$$R_1(0) = 0,\ R_2(0) = 1,\ R_3(0) = 0. \quad (2.10)$$

The differential equations satisfied by $Q_1(z)$, $Q_2(z)$, and $Q_3(z)$ (derived in an analogous fashion) are

$$Q_1'(z) = [d(z) + c(z)R_1(z)]Q_1(z), \quad (2.11)$$

$$Q_2'(z) = c(z)Q_1(z)R_2(z), \quad (2.12)$$

$$Q_3'(z) = [c(z)R_3(z) + f(z)]Q_1(z), \quad (2.13)$$

with the suitable initial conditions

$$Q_1(0) = 1,\ Q_2(0) = 0,\ Q_3(0) = 0. \quad (2.14)$$

It is easy to show that the above process does indeed solve the original linear problem. Define functions $\bar{u}(z)$ and $\bar{v}(z)$ by the relations

$$\bar{u}(z) = R_1(z)\bar{v}(z) + \alpha R_2(z) + R_3(z), \quad (2.15)$$

$$\beta = Q_1(z)\bar{v}(z) + \alpha Q_2(z) + Q_3(z), \quad (2.16)$$

where $R_1(z)$, $R_2(z)$, $R_3(z)$, $Q_1(z)$, $Q_2(z)$, and $Q_3(z)$ satisfy the differential equations (2.7–2.14). By differentiating in (2.15) and (2.16) and using (2.7–2.14), we see that the functions $\bar{u}(z)$ and $\bar{v}(z)$ satisfy (2.1–2.3).

Thus our algorithm involves solving (2.7–2.14) and then using (2.4) and (2.5) to get $u(z)$ and $v(z)$. At first sight it appears that we are going to a great deal of effort; however, as we shall see in the next section, the equations defined by (2.7–2.14) are quite stable for many problems which are unstable as classical initial value problems. In addition, we see that once we have solved (2.7–2.14), we can solve (2.1) and (2.2) for various values of α and β by using (2.4) and (2.5).

Depending on the form of the initial conditions in (2.3), we may wish to write (2.4) and (2.5) in the form

$$v(z) = S_1(z)u(z) + \beta S_2(z) + S_3(z), \quad (2.17)$$

$$\alpha = T_1(z)u(z) + \beta T_2(z) + T_3(z). \quad (2.18)$$

The differential equations satisfied by the S and T functions are

$$-S_1'(z) = c(z) + [a(z) + d(z)]S_1(z) + b(z)S_1^2(z), \quad (2.19)$$

$$-S_2'(z) = [d(z) + b(z)S_1(z)]S_2(z), \quad (2.20)$$

$$-S_3'(z) = [d(z) + b(z)S_1(z)]S_3(z) + e(z)S_1(z) + f(z), \quad (2.21)$$

$$-T_1'(z) = [a(z) + b(z)S_1(z)]T_1(z), \quad (2.22)$$

$$-T_2'(z) = b(z)T_1(z)S_2(z), \quad (2.23)$$

$$-T_3'(z) = [b(z)S_3(z) + e(z)]T_1(z), \quad (2.24)$$

with the initial conditions

$$S_1(0) = 0,\ S_2(0) = 1,\ S_3(0) = 0, \quad (2.25)$$

$$T_1(0) = 1,\ T_2(0) = 0,\ T_3(0) = 0. \quad (2.26)$$

In order to apply the above technique to second-order equations, we first convert the second-order equation into two first-order equations and then apply the method of invariant imbedding as described above.

3. Numerical results

In order to illustrate the advantage of the invariant imbedding over the classical technique, we shall consider two examples of unstable initial value problems.

Example 1: Our first example (also solved in Greenspan (1967) using boundary value techniques) is

$$y''(z) - (z^2 - 1)y(z) = 0, \quad (3.1)$$

$$y(0) = 1,\ y'(0) = 0. \quad (3.2)$$

The general solution of (3.1) is given by

$$y(z) = Ae^{-z^2/2} + Be^{-z^2/2}\int_0^z e^{t^2}dt \quad (3.3)$$

and with the initial conditions (3.2), the desired solution

Table 1

z	$y(z)$ EXACT	INVARIANT IMBEDDING	CLASSICAL INITIAL VALUE	BACKWARD INTEGRATION
0	1·0	1·0	1·0	1·0
1	6·065307 − 01	6·065307 − 01	6·065307 − 01	6·065306 − 01
2	1·353353 − 01	1·353353 − 01	1·353353 − 01	1·353353 − 01
3	1·110900 − 02	1·110900 − 02	1·110900 − 02	1·110900 − 02
4	3·354626 − 04	3·354626 − 04	3·354648 − 02	3·354627 − 02
5	3·726653 − 06	3·726653 − 06	3·879808 − 06	3·726653 − 06
6	1·522998 − 08	1·522998 − 08	3·103631 − 05	1·522998 − 08
7	2·289735 − 11	2·289735 − 11	1·761642 − 02	2·289736 − 11
8	1·266417 − 14	1·266417 − 14	2·780004 − 01	1·266417 − 14
9	2·576757 − 18	2·576758 − 18	1·212432 + 05	2·576759 − 18
10	1·928750 − 22	1·928752 − 22	1·456040 + 09	1·928756 − 22

is

$$y(z) = e^{-z^2/2}, \tag{3.4}$$

which is clearly the minimal solution. Thus standard initial value techniques will have difficulty in accurately approximating the solution over an interval of any appreciable length. Also, since $e^{-z^2/2}$ is dominant with decreasing z, a backward integration scheme should be feasible.

In order to apply the invariant imbedding approach, we first convert (3.1) into the two first-order equations

$$u'(z) = v(z), \tag{3.5}$$

$$-v'(z) = -(z^2-1)u(z), \tag{3.6}$$

$$u(0) = 1, v(0) = 0, \tag{3.7}$$

where $u(z) = y(z)$ and $v(z) = y'(z)$. There are infinitely many ways to convert a second-order equation into a pair of first-order equations. It is possible that some ways may be better than others for numerical computation.

The form of the initial conditions in (3.2) and the coefficients in (3.5) and (3.6) indicate that the relations (2.17) and (2.18) are most convenient and, since $e(z)$ and $f(z)$ are identically zero, the functions $S_3(z)$ and $T_3(z)$ are identically zero. In addition, since $\beta = v(0) = 0$, there is no need to solve for $S_2(z)$ and $T_2(z)$. Thus our algorithm for this example becomes

$$-S_1'(z) = -(z^2-1) + S_1^2(z), S_1(0) = 0, \tag{3.8}$$

$$-T_1'(z) = S_1(z)T_1(z), T_1(0) = 1, \tag{3.9}$$

or

$$-S_1'(z) = -(z^2-1) + S_1^2(z), S_1(0) = 0, \tag{3.10}$$

$$u'(z) = S_1(z)u(z), u(0) = 1. \tag{3.11}$$

For the backward integration scheme, we take

$$y(Z) = 1, y'(Z) = 0, Z \geqslant 10, \tag{3.12}$$

and integrate backward from $z = Z$ to $z = 0{\cdot}0$ and normalise all tabulated values by $y(0)$. Repeat for $Z' > Z$ and compare answers. However, unless the asymptotic form of the solution is known, the backward integration scheme may be difficult to apply. For example, a suitable set of starting values such as (3.12) may not be easy to obtain and, in addition, the process may have to be repeated for several values of Z'.

The original problem (3.1–3.2), the second of the invariant imbedding algorithms (3.10–3.11), and the backward integration scheme were solved on a CDC–6600 using a fourth-order Runge-Kutta integration scheme with $\Delta z = 0{\cdot}005$. The results are displayed in **Table 1**, and clearly demonstrate the advantage of the invariant imbedding and the backward integration schemes.

Example 2: Our last example was discussed very briefly in Fox and Mitchell (1957). The problem is

$$y'' - 11y'(z) - 12y(z) + 22e^z = 0, \tag{3.13}$$

$$y(0) = 1, y'(0) = 1, \tag{3.14}$$

which we write in the form

$$u'(z) = v(z), \tag{3.15}$$

$$-v'(z) = -12u(z) - 11v(z) + 22e^z, \tag{3.16}$$

$$u(0) = 1, v(0) = 1. \tag{3.17}$$

The general solution is given by

$$y(z) = Ae^{-z} + Be^{12z} + e^z, \tag{3.18}$$

and the initial conditions yield the solution

$$y(z) = e^z. \tag{3.19}$$

This problem is difficult to handle with any initial value technique on the original equation, since the exact solution e^z grows at a rate between e^{-z} and e^{12z}. With forward integration, e^{12z} will eventually take over while e^{-z} grows on backward integration overtaking e^z, which decreases on backward integration.

Our relations in this case will be (2.4) and (2.5), and this leads to the equations defined by (2.7–2.14). The results of solving (3.13–3.14) and (2.7–2.14) are displayed in **Table 2**. Although both techniques are beginning to show deterioration, the invariant imbedding is considerably more stable. This particular problem would

Table 2

z	$y(z)$ EXACT	SINGLE PRECISION INVARIANT IMBEDDING	DOUBLE PRECISION INVARIANT IMBEDDING	SINGLE PRECISION CLASSICAL INITIAL VALUE	DOUBLE PRECISION CLASSICAL INITIAL VALUE
0·0	1·0	1·0	1·0	1·0	1·0
0·2	1·221403	1·221403	1·221403	1·221403	1·221403
0·4	1·491825	1·491825	1·491825	1·491825	1·491825
0·6	1·822119	1·822119	1·822119	1·822119	1·822119
0·8	2·225541	2·225541	2·225541	2·225539	2·225539
1·0	2·718282	2·718282	2·718282	2·718258	2·718258
1·2	3·320117	3·320118	3·320117	3·319851	3·319851
1·4	4·055200	4·055211	4·055200	4·052266	4·052266
1·6	4·953032	4·953166	4·953035	4·920689	4·920691
1·8	6·049647	6·051146	6·049675	5·693119	5·693140
2·0	7·389056	7·407488	7·389360	3·458983	3·459217

probably be best solved by using an implicit finite difference boundary technique.

5. Conclusions

The process described above may also be applied to N-dimensional equations. For a discussion of the application of invariant imbedding to N-dimensional systems, the reader is referred to Scott (1969).

We have shown that the method of invariant imbedding may sometimes be used to convert unstable initial value problems into an equivalent stable initial value problem, and that the solutions for various initial values involve no extra integration but only algebraic manipulation.

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Book review

Machine Intelligence, Vol. 5, Edited by B. Melzer and D. Michie, 588 pages. (*Edinburgh University Press*, £7·00)

This volume is the proceedings of the Fifth Annual Machine Intelligence Workshop held at Edinburgh University in the autumn of 1969. Readers of the proceedings of previous Workshops will know that the term 'Machine Intelligence' is taken to encompass a wide range of computing activities. What is important to readers of *The Computer Journal* is that these Workshops have become one of the most notable platforms for presenting the latest advances in the Theory of Programming. It is a strange fact that in the vast number of computing meetings held all over the world papers on the fundamentals of programming are scarce. Yet it is on programming that most computing activity basically depends.

There are four accepted ways of approaching programming theory—via recursive function theory, algebra, set theory or logic. All four methods were represented in this Workshop, which definitely counts as a vintage year. R. Milner associates recursively enumerable sets with program schemas, he shows that various forms of equivalence between schemas can be examined by comparing these sets. P. J. Landin gives a new, and original, treatment of program execution by using Universal Algebra. The successive states of a computation caused by one machine operation after another, and the succession of instructions in the program which cause the machine operation are linked in an interesting way, which Landin illustrates by an ingenious analogy. R. M. Burstall gives an axiomatic specification of a sub-set of ALGOL 60. Here the constructs and data operations of the language are described by axioms. Such descriptions of the semantics of programming languages are likely to become of practical significance in the future. Two authors who have done much to pioneer the logical description of the properties of programs, Z. Manna and J. McCarthy, formalise the properties of recursive programs and show the effect of different evaluation rules. D. Park in an important new paper shows how the functions computed by programs are associated with the recursive definition of sets. His approach uses the step-by-step nature of program execution to carry out inductive proofs of program properties. It is the step-by-step action of computation which so sharply distinguishes programming and mathematical notation, here is mathematics which goes to the heart of the problem. This paper must be read.

While the papers on programming alone make this book worth buying there are, in fact, 24 further papers covering topics like theorem proving, heuristics, and pattern recognition. There is space to mention only a few of the contributions. K. A. Paton and D. Rutovitz give detailed reports of the progress of work being done on a project for automatic chromosome analysis, which is sponsored by the Medical Research Council. Progress is steady, and as in previous reports from this group, it is seen that success is due to carefully adapting techniques to the specific problem. The Department of Machine Intelligence at Edinburgh itself is much in evidence, and their strong interest in heuristics has now moved towards feedback situations involving robots. They seem to be converging on the related problems from many angles, and are using techniques ranging from logic to the construction of mechanical arms. Readers interested in Theorem Proving will have to look at this book for themselves, it will be well worthwhile. An additional pleasure is the opportunity to read a paper written by A. M. Turing in 1947, now published for the first time, entitled 'Intelligent Machinery'. This paper gives a sobering measure of progress in 23 years, but is also inspiring.

J. J. FLORENTIN (London)