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RAMON E. MOORE

Automatic Local Coordinate Transformations to Reduce the Growth of Error Bounds in Interval Computation of Solutions of Ordinary Differential Equations

1: INTRODUCTION

It is the purpose of this paper to consider some local coordinate transformation techniques which can be carried out automatically by the computer for general systems of first order analytic differential equations and which will reduce the growth of interval error bounds produced by the method of successive expansions in Taylor series with interval remainder.

In a previous work by the author (Moore [65]), a technique based on computations by the computer with interval numbers, i.e. closed intervals of real numbers, was presented. Using the technique, a digital computer can determine intervals containing exact values of solutions to systems of ordinary differential equations.

The technique consists of successive expansions in Taylor series to a certain number of terms with the remainder bounded by the computer over certain intervals which it also determines. As a result, the machine computation automatically produces intervals containing exact solution values for all solutions beginning in given initial intervals.

A practical procedure for programming the recursive generation of Taylor coefficients was also presented in Moore [65]. The procedure consists in displaying the expressions for the first derivatives given by the system of differential equations as a finite sequence of products, sums, quotients, roots and elementary functions - all of which have general recursion formulas for their k th Taylor coefficients in terms of the coefficients of lower order. The chain rule of Leibniz, $\frac{dX(Y(t))}{dt} = X'Y'$, permits an assembly of the resulting set of recursion formulas into a program for the computation of the general Taylor coefficients of the solution. See also Fehlberg [63, 64, 64a], and Steffensen [56]. Thus we will feel free in this paper to consider computational schemes requiring truncated Taylor series expansions.

An operational program for the IBM 7094 computer which uses all these techniques has been written and is available from SHARE [65].

In principle, by going to multiple precision or long enough word length on the computer, the bounding intervals containing an exact solution value at a particular value of the independent variable can be made of arbitrarily small width for a particular solution with exactly known initial values.

If the real n-vector $y = y(t, y_0)$ satisfies

$$dy/dt = f(t, y)$$

$$y(t_0, y_0) = y_0$$

for some interval of values of t, then the technique of Moore [65] produces an interval n-vector valued function $Y(t, Y_0)$ such that if y_0 is in* Y_0, then $y(t, y_0)$ is contained* in $Y(t, Y_0)$.

The requirement of analyticity of f is a local one. We need to be able to expand in Taylor series along the solution curves $y(t, y_0)$. In addition the components of f must be expressible by compositions and rational combinations of elementary functions or functions which can themselves be defined by differential equations of admissible type. In effect, we need programmable expressions for the first derivatives of all quantities appearing in the system.

If we denote by $Y^{(n)}(t, y_0)$ the result obtained by the procedure with n place binary arithmetic, then the maximum of the widths of the components of $Y^{(n)}(t, y_0)$ for fixed t will be $O(2^{-n})$.

On the other hand, for fixed n, the interval components of $Y^{(n)}(t, y_0)$ will increase with t. This follows from the fact that the width of the sum of two intervals is the sum of the widths. Since $[a, b] + [c, d] = [a + c, b + d]$, it follows that $(b + d) - (a + c) = (b - a) + (d - c)$. Since our interval result has the form $Y(t, y_0) = Y(t_0, y_0) + (t - t_0) F$ with F consisting of the terms in the series involving successive total derivatives of f, it follows that the components of $Y(t, y_0)$ increase in width as t increases. The contribution to the width of a component of F from the remainder term in the Taylor series is of the form $k(t - t_0)^9$ in our program cited, since we carry expansions to nine terms. Therefore if we carry out a new expansion before $t - t_0$ gets too large then the rate of growth from this source can apparently be kept very small.

Of course, this is not to say that the contribution of the remainder terms to the widths of bounding intervals produced by the program cannot be diminished by various refinements of the schemes

* Component by component.

involved such as more detailed procedures for choosing the number of terms to be used in the expansions depending in some way on the particular set of equations being solved, etc.

The situation is much more involved when we consider interval solutions beginning with intervals of initial values Y_0, and for either interval or exact initial values when we consider the actual growth of interval widths from all sources during successive expansions of an interval solution carried out with fixed n, i.e. a fixed number of binary places in the arithmetic.

We shall see shortly that the very form in which we seek to represent solutions, namely interval vector valued functions $Y(t, y_0)$, must necessarily cause a certain excess growth in interval widths in connection with any scheme of successive expansions, no matter what the details of the scheme. We will even admit the possibility of iterative finishing procedures for sharpening the bounding interval functions over each interval of expansion. In fact, we shall indicate next a few such iterative procedures. After that, we shall describe precisely the problem with which we are concerned in this paper, and indicate the general approach to its solution to be discussed in the next sections.

1.1 The method of Chaplygin

Henrici [62], p. 106, gives several references to papers on a method due to Chaplygin, (see also, Chaplygin [19], Chaplygin [48], Petrov [45], Savarensky [45], Baranov [64], Gendzhoian [64], Pak and Chichkin [64], Azbelev [62]), which concerns the iterative improvement of two sided approximations to solutions of differential equations.

In the method of Chaplygin for a single equation, $y' = f(x, y)$, one begins with a pair of curves constituting upper and lower bounding curves $U(x)$, $L(x)$ to the solution $y(x)$ defined over a definite range of values of x, say $[x_0, x_1]$ which passes through the point (x_0, y_0). Then

$$L(x) < y(x) < U(x) \quad \text{for} \quad x \text{ in } [x_0, x_1].$$

Such a pair of bounding curves could be found to begin with by the computer using the above mentioned program SHARE [65], or by hand using the interval expansion method of Moore [65]. More simply, a rough pair could be determined by putting

$$L(x) = y_0 + (f(x_0, y_0) - b)(x - x_0)$$

$$U(x) = y_0 + (f(x_0, y_0) + b)(x - x_0)$$

with b and x_1 chosen so that $|f(x,y) - f(x_0,y_0)| < b$

for x in $[x_0, x_1]$

and y in $[y_0+(f(x_0,y_0)-b)(x_1-x_0),\ y_0+(f(x_0,y_0)+b)(x_1-x_0)]$.

A new pair of bounding curves $L_1(x)$, $U_1(x)$ is "constructed" such that

$$L(x) < L_1(x) < y(x) < U_1(x) < U(x)$$

for x in $[x_0, x_1]$ by a method to be described presently. The process is repeated and it can be proved that (ignoring round-off) the process is error squaring and hence rapidly convergent if $L(x)$ is close enough to $U(x)$ to being with.

In order for the procedure to continue to provide upper and lower bounding curves to the solution it is necessary to assume that the function $f(x,y)$ regarded as a surface in 3-space is convex in y for each x whenever (x,y) lies in the region R_1 determined by x in $[x_0, x_1]$ and y between $L(x)$ and $U(x)$.

One approximates f by a surface f_1 generated by tangent lines parallel to the y,f plane on one side and he also approximates f by a surface f_2 generated by chords on the other side. He then "solves" the linear differential equations

$$U_1' = f(x, L(x)) + \frac{\partial f}{\partial y}(x,\ L(x))(U_1 - L(x))$$

$$L_1' = f(x, L(x)) + \frac{f(x, U(x)) - f(x, L(x))}{U(x) - L(x)}(L_1(x) - L(x))$$

for $L_1(x)$ and $U_1(x)$, x in $[x_0, x_1]$.

Assuming now that $\frac{\partial^2 f}{\partial y^2} < 0$ in R_1 and that R_1 is not too large, it is shown (Chaplygin [19]) that the process is convergent. The error squaring results from the fact that the two surfaces

$$f_1(x,y) = f(x, L(x)) + \frac{\partial f}{\partial y}(x, L(x))(y - L(x))$$

$$f_2(x,y) = f(x, L(x)) + \frac{f(x, U(x)) - f(x, L(x))}{U(x) - L(x)}(y - L(x))$$

depart quadratically from f in the quantity $y - L(x)$. Just as in

Newton's root finding method the tangent lines depart quadratically from the graph of the function.

Various more complicated sufficient conditions occur with systems of more than one equation and of course computationally one still has the problem of actually or approximately solving the linear equations which arise at each stage of the iteration. Nevertheless, the method could conceivably be used to design a fairly general program for automatically narrowing somewhat the interval solutions obtained by the method of Moore [65].

For other work on two sided approximations based on convexity or on the local constancy of sign of various expressions in higher derivatives, see: Piaggio [19], Gorn and Moore [53], Gorbunov and Shakov [63].

1.2 Picard iteration

A much more slowly convergent procedure for the iterative improvement of interval bounds but a simpler and more general one can be based on successive substitutions in an equivalent system of integral equations. This method amounts to an interval version of the well-known Picard iteration.

Suppose we obtain an interval vector solution $Y(x)$ containing the exact vector solution $y(x)$ to the differential system written in vector form $y' = f(x, y)$ for x in some interval $[x_0, x_1]$, with $y(x_0) = y_0$. Then $y(x)$ satisfies the equivalent vector integral equation

$$y(x) = y_0 + \int_{x_0}^{x} f(x', y(x'))\,dx' .$$

Since $y(x)$ is contained in $Y(x)$, we will have

$$y(x) \in Y(x_0) + \int_{x_0}^{x} f(x', Y(x'))\,dx' \quad \text{if} \quad y_0 \in Y(x_0) .$$

Consider the sequence of interval vector functions defined by

$$Y^{(1)}(x) = Y(x)$$

$$Y^{(n+1)}(x) = Y(x_0) + \int_{x_0}^{x} f(x', Y^{(n)}(x'))\,dx .$$

We can see that if $\max_i \sum_j \left|\frac{\partial f_i}{\partial y_j}\right| < K$ for $x \in [x_0, x_1]$, $y(x) \in Y(x)$,

then denoting the maximum width of the components of an interval vector V by $w(V)$, we will have

$$w(Y^{(n+1)}(x)) \leq w(Y(x_0)) + \int_{x_0}^{x} K\, w(Y^{(n)}(x'))\, dx'$$

and

$$w(Y^{(n+1)}(x)) \in w(Y(x_0)) + K(x-x_0) \max_{x' \in [x_0, x]} w(Y^{(n)}(x')) .$$

Hence the sequence of interval functions $Y^{(1)}, Y^{(2)}, \ldots$ (each of which contains the solution function f for x in $[x_0, x_1]$) will be a nested sequence converging to the solution function provided that $K(x_1 - x_0) < 1$, (again ignoring round-off). Notice that even in case $K(x_1 - x_0) < 1$, the iteration may not reduce the width $w(Y^{(n)}(x))$ below $\frac{1}{1 - K(x - x_0)}\, w(Y(x_0))$.

In order to make this procedure work computationally, it is of course necessary to devise accurate means for evaluating the integrals of interval functions which occur in each stage of the iteration. Such techniques have been discussed in section 7 of Moore [65].

1.3 Dynamical systems and flows

Even with the possibility of iterative improvement of error bounds over each interval of expansion by methods such as those above, there is a source of growth of the widths of bounding intervals which requires an examination of the nature of differential systems and their solutions for its understanding and possible control.

An autonomous * system of n first order differential equations is also called a dynamical system. The equations define a vector field on E_n, euclidean n-space. If $dy/dt = f(y)$ and f is a mapping of E_n (or an open set in E_n) into E_n then the system can be though of as defining a motion or a "flow" of the points y of the "phase space". A point y_0 moves during time t_1 to a point $y(t_1, y_0)$ and from there during time t_2 to the point $y(t_2, y(t_1, y_0)) = y(t_1 + t_2, y_0)$.

In this way the flow in phase space can be viewed as a one parameter continuous group (or a local group) of transformations of the phase space. For each value of the parameter t in an open real

* "autonomous" means f does not depend explicitly on t. This is not an essential restriction since, of course, $y_i' = f_i(t, y_1, \ldots, y_n)$, $(i = 1, 2, \ldots, n)$ in E_n is equivalent to the autonomous system $y_i' = f_i(y_{n+1}, y_1, \ldots, y_n), (i = 1, 2, \ldots, n)$, $y_{n+1}' = 1$ in E_{n+1}.

interval we have a transformation $T(t)$ of the points y_0 of the phase space indicated by $y = y(t, y_0) = T(t)[y_0]$. Thus, $T(t_1+t_2)[y] = T(t_1)[T(t_2)[y]]$.

On the other hand, for fixed y_0, regarding $y(t, y_0)$ as a mapping of the space of the parameter t which we will take as the real line* or an open interval, we can consider the image of the mapping to be the "orbit" of the point y_0 under group of transformations, or the "trajectory" of a particle beginning at y_0 or the stream line of the flow through y_0.

If we determine by some approximation method that at t_1 the point $y(t_1, y_0)$ lies in the interval vector $Y(t_1, y_0)$ then we have in effect computed a rectangular region represented by the vector of intervals $Y(t_1, y_0)$ which contains the point $y(t_1, y_0)$. This rectangular region, furthermore has sides parallel to the y_i coordinate axes.

We will call such a region in E_n, a box. Thus a box is a set of points $y = (y_1, y_2, \ldots, y_n)$ in E_n consisting of the cartesian product of n closed real intervals; i.e., a box is representable by an ordered n-tuple of intervals $Y = (Y_1, Y_2, \ldots, Y_n)$, i.e., an interval vector. A point y is in the box Y if y_i lies in the interval Y_i for each $i = 1, 2, \ldots, n$.

The procedure of successive expansions with interval error bounding leads to boxes $Y_1, Y_2, \ldots$ such that $y(t_1, y_0)$ is in Y_1 for every y_0 in Y_0; $y(t_2, y_1)$ is in Y_2 for every y_1 in Y_1; etc., etc. Therefore, we will have $y(t_2 + t_1, y_0)$ contained in Y_2; $y(t_3 + t_2 + t_1, y_0)$ contained in Y_3; etc., etc.

* In the study of solutions of differential systems in the neighborhood of algebraic singular points of f an extension of the domain of the variable t to the complex field, which is algebraically closed, is exceedingly fruitful. For example, in the vast and beautiful computational study carried out at the Copenhagen Observatory on the restricted three body problem by Stromgren [35], complex transformations were used to continue analytically numerical solutions from collisions to ejections. Besides, these complex transformations were useful in improving accuracy even for near collisions. In these studies, Stromgren and his associates at the Copenhagen Observatory, over some decades, found and graphed a very large number of complete families of periodic solutions of fascinating and significant variety, without the benefit of modern computing machines.

In the present paper, however, we will content ourselves with concern for real systems with f analytic in regions of interest. The equations for the restricted three body problem are regular except at the two gravitationally attracting bodies acting on the small third body whose motion the equations describe. Thus, we do not exclude systems such as the resticted three body equations, but only must confine ourselves to regions which do not include singularities of f.

On the other hand, under the flow itself a box Y is carried after time t into the set of points

$$y(t,Y) = \{y(t,p) | p \in Y\}$$

which will in general not remain a box except for a few simple flows such as rigid translations of the whole phase space in a fixed direction and spherically symmetrical expansion of the whole space about the center of the box Y. Usually, a flow will rotate and distort a box.

An example will help to make clear what the problem is. Consider the system

$$\begin{aligned} dy_1/dt &= y_2 \\ dy_2/dt &= -y_1 \end{aligned} \qquad (1)$$

Let $T(t)$ be the transformation of the plane represented by the matrix

$$T(t) = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix}$$

then we have

$$y(t, y_0) = T(t)\, y_0$$

and

$$y(t,Y) = \{y(t,p) | p \in Y\} = \{T(t)p | p \in Y\} .$$

Figure 1 illustrates the "rotated box" $y(\pi/4, Y_1)$

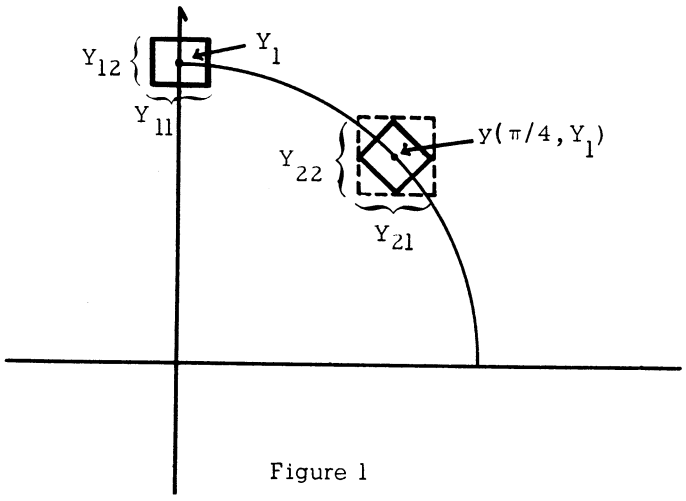

Figure 1

Clearly the smallest box (with sides parallel to the y_1, y_2 coordinate axes) containing $y(\pi/4, Y_1)$ is that indicated by the dotted rectangle consisting of the interval vector

$$Y_2 = \begin{pmatrix} Y_{21} \\ \\ Y_{22} \end{pmatrix} = \begin{pmatrix} \cos \pi/4 & \sin \pi/4 \\ \\ -\sin \pi/4 & \cos \pi/4 \end{pmatrix} \begin{pmatrix} Y_{11} \\ \\ Y_{12} \end{pmatrix}$$

or

$$Y_2 = \begin{pmatrix} Y_{11}/\sqrt{2} + Y_{12}/\sqrt{2} \\ \\ -Y_{11}/\sqrt{2} + Y_{12}/\sqrt{2} \end{pmatrix}$$

Supposing the intervals Y_{11} and Y_{12} are of equal width w, then the widths of Y_{21} and Y_{22} will be $\sqrt{2}w$. If we should carry out the expansion procedure at steps of $\pi/4$ ($= .78\ldots$) in t with interval bounding, we would have an increase in the widths of bounding boxes amounting at least to multiplication by $(\sqrt{2})^8 = 16$ per revolution of the solution.

By decreasing the steps to small Δt in this example the increase in widths of bounding boxes after m steps will still be a factor close to $e^{m\Delta t}$. Per revolution, $m\Delta t = 2\pi$; $e^{2\pi}$ is around 500. Thus the trouble does not go away by using smaller steps between expansions.

The program cited above, (SHARE [65]), actually repeated expansions for the example above at intervals of about 0.54 in t and widths of bounding intervals increased by a factor of about 500 per revolution.

In differential systems of higher dimension the growth of bounding intervals due to this phenomenon can be still more pronounced considering, for example, that the diagonal of the unit n-cube has length $\sqrt{n}$.

In the example (1) connected with figure 1, we know, of course, that the solution curves are circles about the origin so that by introduction of polar coordinates, the integral curves $y_1^2 + y_2^2 =$ const. are parametrized by a single variable θ satisfying a single first order equation $d\theta/dt = 1$. An "integral" of a differential system $\frac{dy}{dt} = f(y)$ in E_n is a non-constant real mapping of E_n, H, satisfying

$$\frac{dH}{dt}\Big|_{\substack{= \\ \text{along} \\ \text{solutions}}} \frac{\partial H}{\partial y_1} f_1 + \ldots + \frac{\partial H}{\partial y_n} f_n = 0 .$$

An integral H layers the phase space E_n into n-1 dimensional differentiable manifolds (locally "diffeomorphic" to E_{n-1}) called integral manifolds or integral surfaces. If a point y_0 is on one of these surfaces then the entire trajectory through y_0 lies on the surface, that is $H(y(t, y_0)) = H(y_0)$. In the dynamics of systems of particles, etc., conservation laws (energy, angular momentum, etc.) appear as integrals of the differential equations of motion. From the point of view that a dynamical system defines a flow in the phase space, these integral surfaces can be thought of as "stream surfaces". If a suitable parametrization (coordinatization) of the manifolds can be found, the dimension of the flow can be reduced and the source of growth of error bounds under discussion will, in principle, be diminshed.

T. M. Cherry [24], has shown for analytic differential systems how to obtain series representations (in powers of the components of a point on the surface) locally for a complete set of n - 1 integral surfaces in the neighborhood of a given point in the phase space. By intersecting these integral surfaces, i. e. by considering their defining equations together as a "simultaneous" system of equations, the motion of a point can be locally approximated (for some interval in t) arbitrarily closely by solving a single first order differential equation. An approach to the control of the growth of interval error bounds could conceivably be based upon Cherry's local expansions of integral surfaces, using, say, the first two terms in each expansion to define a set of "integral coordinates". Various difficulties appear, however, such as the inversion of non-linear transformations in E_n and the fitting together of successive local integral surfaces in such a way as to maintain a simple formalism (so that a tractable computational algorithm can be derived).

In celestial mechanics and in the study of satellite orbits and space probe trajectories a great deal of success has been had considering the equations of motion as perturbations of the two-body equations. The coefficients of the integral curves (conic sections) of the two-body problem, for example, can be taken as coordinates and differential equations for their time variation derived so that the motion being studied (including, perhaps, effects of several attracting bodies, "oblateness" of the earth, atmospheric "drag", etc.) is approximated locally by solutions to the two body problem. Among the many such choices of sets of variables used in this work, there must be many which would result in smaller growth of interval error bounds via the solution of their derived differential equations than that resulting from direct use of the inertial cartesian coordinates. Certainly the long, successful history of work on motions in the solar system is filled with transformations of variables accomplishing a great variety of objects.

1.4 Local coordinate transformations

The idea we will investigate in the succeeding sections of this paper is to seek algorithms which can be carried out by the computer for producing time dependent transformations of coordinates $y = T(t, z)$ (so that at each t we have a local z coordinate system) for a given differential system $y' = f(y)$ using properties of the system at points y_1 near a particular solution $y(t, y_0)$ such that the derived differential system

$$z' = \left(\frac{\partial T}{\partial z}\right)^{-1} \{f(T(t, z)) - \frac{\partial T}{\partial t}\}$$

(or its autonomous equivalent in E_{n+1}) defines a flow $z(t, y_0, y_1)$ which tends to preserve small boxes (i.e. with y_1 close to $y(t, y_0)$) in the z coordinate space. Thus we wish to have $z(t, y_0, Y_1)$ remain close to a box for a small box Y_1 with center at y_0. At any rate if we apply the method of successive interval expansions in Taylor series with interval remainder to the derived differential system for z and the resulting interval bounds $Z(t)$ in the moving z coordinates grow slowly enough, then the resulting interval bounds $Y(t)$, (boxes), in the original y coordinates obtained by bounding $T(t, Z(t)) \subset Y(t)$ will have a reduced rate of growth compared to those obtained directly from successive expansions with interval remainder for the original differential system $y' = f(y)$.

We will consider the problem from a variety of related points of view and derive various transformations mainly of the form

$$y(t, y_1) = y^*(t, y_0) + S(t, y_0) z(t, y_0, y_1)$$

where $y^*(t, y_0)$ is a real approximation to $y(t, y_0)$ and $S(t, y_0)$ is a non-singular real linear transformation. If we determine a box valued function $Z(t, y_0, Y_1)$ by interval solution, (Moore [65]), of the derived differential system in z, using $z(0, y_0, Y_1) = Y_1 - y_0$, (if $S(0, y_0) = I$, the identity transformation), such that

$$z(t, y_0, Y_1) \subset Z(t, y_0, Y_1),$$

then by interval evaluation we can compute a box

$$Y(t, Y_1) = y^*(t, y_0) + S(t, y_0) Z(t, y_0, Y_1)$$

such that $y(t, y_1)$ is in $Y(t, Y_1)$ for every y_1 in Y_1. Choosing $y^*(t_1, y_0)$ for some $t_1 > t_0$ as a new y_0 we can continue the process by determining a new $y^*(t, y_0)$ and $S(t, y_0)$ to be used during the next interval in t of expansion of z and then continuing the interval solution of the z differential system with $Z(t_1, y_0, Y_1)$ as the new initial z box for the next expansion. Thus the form of the transformation from z to y will remain unchanged

as t increases as will the form of the differential system for z at each new expansion point $t_0, t_1, t_2, \ldots$; however we will have new coefficients in the expressions for y^*, S and in the differential equation for z. Since we are in effect solving a new initial value problem in z in each interval of expansion in t, and since the final value of z in one t expansion interval becomes the initial value of z in the next expansion interval, there will be no difficulty concerning discontinuities in the Taylor coefficients, for these will always be computed interior to the expansion interval.

2. THE GEOMETRIC APPROACH OF N. S. HAWLEY

An approach suggested to the author by Newton Hawley is motivated by geometrical concepts such as circles of curvature, intrinsic coordinates, etc.

2.1 The circle of curvature method.

Consider the dynamical system $dy/dt = f(y)$ in E_n again and denote by y_0' the vector $f(y_0)$ and by y_0'' the vector $(d/dt)f(y)\big|_{y_0} = \frac{\partial f}{\partial y} f(y)\big|_{y=y_0}$. We fix y_0 and consider the curve $y(t, y_0)$.

Suppose that y_0' and y_0'' are not collinear. (If y' and y'' are collinear over an interval of values of t along a trajectory $y(t, y_0)$ for an analytic differential system, then the entire trajectory lies on a straight line). Then y_0' and y_0'' determine a plane through y_0, the so-called "osculating" plane to the trajectory $y(t, y_0)$ through y_0. Using the notation (u, v) for the inner product of two vectors u, v, $(u, v) = u_1v_1 + \ldots + u_nv_n$, we can represent the so-called "circle of curvature" to $y(t, y_0)$ at y_0 as a circle in the y_0', y_0'' plane with center at

$$c_0 = y_0 + \rho_0 \frac{n_0}{(n_0, n_0)^{1/2}}$$

and radius

$$\rho_0 = \frac{(y_0', y_0')^{1/2}}{(n_0, n_0)^{1/2}}$$

where

$$n_0 = y_0'' - \frac{(y_0', y_0'')}{(y_0', y_0')} y_0' .$$

Call

$$e_1(0) = \frac{y_0'}{(y_0', y_0')^{1/2}}, \quad e_2(0) = \frac{n_0}{(n_0, n_0)^{1/2}},$$

thus $e_1(0)$, $e_2(0)$ are the unit tangent and normal vectors at y_0. We can approximate the flow $y(t, y_1)$ for y_1 in the neighborhood of y_0 by a uniform rotation $y^*(t, y_1)$ of the phase space in the y_0', y_0'' 2-plane about c_0.

We put

$$(2) \qquad y^*(t, y_1) = c_0 + (y_1 - c_0, e_1(0))\, e_1(t) + (y_1 - c_0, e_2(0))\, e_2(t) + e_3$$

where

$$e_1(t) = (\cos \theta(t))\, e_1(0) + (\sin \theta(t))\, e_2(0)$$

$$e_2(t) = (-\sin \theta(t))\, e_1(0) + (\cos \theta(t))\, e_2(0)$$

$$e_3 = (y_1 - c_0) - (y_1 - c_0, e_1(0))\, e_2(0) - (y_1 - c_0, e_2(0))\, e_2(0)$$

and

$$\theta(t) = \frac{(y_0', y_0')^{1/2}}{\rho_0}\, t .$$

Choosing a z coordinate system carried along by the approximate flow y^*, we can represent trajectory points $y(t, y_1)$ in the original coordinates by

$$(3) \qquad y(t, y_1) = c_0 + z_1 e_1(t) + z_2 e_2(t) + \bar{z}$$

with $y(0, y_1) = y_1$ and

$$z_1(0) = (y_1 - c_0, e_1(0)), \quad z_2(0) = (y_1 - c_0, e_2(0))$$

and with

$$\bar{z}(0) = e_3, \quad (\bar{z}(t), e_1(t)) = (\bar{z}(t), e_2(t)) = 0 .$$

Notice that in two dimensions $\bar{z}(t) \equiv 0$, since in that case e_1, e_2 form a basis for the vector space E_2.

We find that the derived differential system in the z coordinates can be written, (where for brevity, the prime denotes derivative with respect to t),

$$
\begin{aligned}
z_1' &= \theta_0' z_2 + (\bar{z}, e_2)\theta_0' + (f(c_0 + z_1 e_1 + z_2 e_2 + \bar{z}),\ e_1) \\
z_2' &= -\theta_0' z_1 - (\bar{z}, e_1)\theta_0' + (f(c_0 + z_1 e_1 + z_2 e_2 + \bar{z}),\ e_2) \qquad (4) \\
\bar{z}' &= f(c_0 + z_1 e_1 + z_2 e_2 + \bar{z}) + (\theta_0' z_2 - z_1')e_1 - (\theta_0' z_1 + z_2')e_2 .
\end{aligned}
$$

The first two of these are scalar equations and the third is an nth order system for the vector $\bar{z}$ known to lie in the $(n-2)$ space defined by $(\bar{z}(t), e_1(t)) = (\bar{z}(t), e_2(t)) = 0$ at each t. By θ_0', we mean, of course,

$$\theta_0' = \frac{(y_0', y_0')^{1/2}}{\rho_0} .$$

We will illustrate this transformation by applying it to the example (1) above which can also be written in the form

$$y' = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} y . \qquad (1)'$$

For definiteness we put $y_0 = \binom{0}{1}$, then

$$y_0' = \binom{1}{0}, \quad y_0'' = \binom{0}{-1} .$$

We have

$$(y_0', y_0'') = 0$$

$$n_0 = \binom{0}{-1}$$

$$\rho_0 = 1$$

$$e_1(0) = \binom{1}{0}, \quad e_2(0) = \binom{0}{-1}, \quad e_3 = 0$$

$$c_0 = \binom{0}{1} + \binom{0}{-1} = \binom{0}{0} = 0$$

$$\theta(t) = t, \quad \theta_0' = 1$$

$$e_1 = e_1(t) = \cos t \binom{1}{0} + \sin t \binom{0}{-1} = \binom{\cos t}{-\sin t}$$

$$e_2 = e_2(t) = -(\sin t)\binom{1}{0} + \cos t \binom{0}{-1} = \binom{-\sin t}{-\cos t}$$

$$y(t, y_1) = z_1 e_1 + z_2 e_2 + \bar{z}$$

$$y(0, y_1) = y_1 = \begin{pmatrix} y_{11} \\ y_{12} \end{pmatrix}, \quad z_1(0) = y_{11}, \quad z_2(0) = -y_{12}$$

$$\bar{z}(t) \equiv 0$$

$$f(c_0 + z_1 e_1 + z_2 e_2 + \bar{z}) = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \left\{ z_1 \begin{pmatrix} \cos t \\ -\sin t \end{pmatrix} + z_2 \begin{pmatrix} -\sin t \\ -\cos t \end{pmatrix} \right\} = \begin{pmatrix} -z_1 \sin t - z_2 \cos t \\ -z_1 \cos t + z_2 \sin t \end{pmatrix}$$

$$(f, e_1) = -z_2, \qquad (f, e_2) = z_1$$

Therefore the system (4) becomes for the present example the trivial system

$$z_1' = 0$$

$$z_2' = 0$$

$$\bar{z}' = 0 \qquad (\bar{z}(t) \equiv 0) \ .$$

In this case

$$z_1(t) = z_1(0) = y_{11}$$

$$z_2(t) = z_2(0) = -y_{12}$$

for all t, and the flow is completely stopped in the z coordinates.

Thus, in this example, we obtain from (3) a representation (of the solutions ot (1)') of the form

$$y(t, y_1) = y_{11} \begin{pmatrix} \cos t \\ -\sin t \end{pmatrix} - y_{12} \begin{pmatrix} -\sin t \\ -\cos t \end{pmatrix} = \begin{pmatrix} \cos t & \sin t \\ -\sin t & \cos t \end{pmatrix} y_1 .$$

The point here is not that we can solve the system (1)' for this simple example but rather that the transformation from y to z given by (3) can be applied to transform any differential system $dy/dt = f(y)$ into the form (4), (except at inflection points where y_0', y_0'' are collinear) with a resulting reduction at least of the gross primary rotational motion of our bounding boxes.

For systems in which (2) is a good approximation to the flow, some reduction in the growth of interval bounds can be expected through repeated application of the transformation (3) at successive points of expansion.

2.2 Intrinsic coordinates, the attached n-tuple of unit vectors.

Regarding the solution $y(t, y_0)$ passing through y_0 to the system $y' = f(y)$ with f analytic in a neighborhood of $y(t, y_0)$ for each t under consideration as a curve in E_n, we can attach an n-tuple of unit vectors $e_1, e_2, \dots, e_n = e_n(t)$ to the curve at each point in such a way that e_1 is the unit tangent vector, e_2 is a unit vector in the direction of the normal, e_3 is a unit vector in the direction of the binormal, etc. These vectors can be found at a point y on the curve by the Gram-Schmidt orthonormalization of the ordered n-tuple of vectors $(y', y'', y''', \dots, y^{(n)})$, so that e_1 is in the direction y', e_2 is in the direction $y'' - \frac{(y', y'')}{(y', y')} y'$, etc. The vectors $e_1, e_2, \dots, e_n$ form an orthonormal basis for the phase space E_n. Putting $e_1, e_2, \dots, e_n$ as the columns of a matrix $E(t)$, then $E(t)$ becomes (the representation of) an orthogonal transformation for each t and we can approximate the flow of the dynamical system near $y(t, y_0)$ by

$$(5) \qquad y^*(t, y_1) = y(t, y_0) + E(t)E^{-1}(0)(y_1 - y_0) \ .$$

Motivated by this approximation to the flow, we can define a transformation to moving (local) z coordinates by

$$y(t, y_1) = y(t, y_0) + E(t)E^{-1}(0)\, z(t, y_0, y_1) \ .$$

At $t = 0$ we will have $z(0, y_0, y_1) = y_1 - y_0$ and z will satisfy the derived differential system

$$(6) \qquad z' = E(0)E^{-1}(t)\{f(y(t, y_0) + E(t)E^{-1}(0)\, z) - f(y(t, y_0))\}$$
$$- E(0)E^{-1}(t)E'(t)E^{-1}(0)\, z \ .$$

The differentiability of the orthogonal matrix valued function $E(t)$ follows from the supposed analyticity of f along the particular solution curve $y(t, y_0)$.

In principle this transformation should serve very well, for y_1 near enough to y_0, to control the rotation in n-space of bounding boxes in the local z coordinates. However, the computation of $E(t)$, $E'(t)$ in practice requires further approximation and because of the complexity of the dependence of $E(t)$ on f the analysis in the general case of the errors involved is apparently very complicated.

It is interesting to conjecture whether some use could be made of the classification of orthogonal transformations given by Kuiper [62]: [On p. 174]: "With suitable coordinates the matrix of

an orthogonal endomorphism (of E_n) is $\begin{bmatrix} \sigma_1 & & & \\ & \sigma_2 & & \\ & & \ddots & \\ & & & \sigma_m \end{bmatrix}$

with $\sigma_i = 1, -1,$ or $\begin{pmatrix} \cos\varphi_i & \sin\varphi_i \\ -\sin\varphi_i & \cos\varphi_i \end{pmatrix}$ for $i = 1, 2, \ldots, m$ and zeros in all other places."

2.3 Approximating linear systems.

An approach closely related to that just considered in section 2.2 but which leads to more tractable expressions is to approximate the flow satisfying a given dynamical system $y' = f(y)$ in E_n by one satisfying a linear system with constant coefficients.

$$(y^*)' = Ay^* + b \tag{7}$$

with A and b to be chosen such that

$$\begin{aligned} y_0'' &= Ay_0' \\ y_0''' &= Ay_0'' \\ &\cdots\cdots \\ y_0^{(n+1)} &= Ay_0^{(n)} \\ b &= y_0' - Ay_0 \end{aligned}$$

for then if we put

$$y^*(0, y_0) = y_0$$

we will have

$$y^*(t, y_0) = y_0 + ty_0' + t^2y_0''/2 + \ldots + t^n y_0^{(n)}/n! + O(t^{n+1}) .$$

Thus the approximate flow is made to agree in its Taylor expansion to terms of order t^n with the flow defined by the given dynamical system in E_n.

Denote by Y_0 the matrix whose columns are the vectors $y_0', y_0'', \ldots, y_0^{(n)}$ and by Y_0' the matrix whose columns are $y_0'', y_0''', \ldots, y_0^{(n+1)}$. Then $Y_0' = AY_0$ and we can determine A by $A = Y_0'Y_0^{-1}$. The matrix Y_0 will be singular for example if the trajectory $y(t, y_0)$ lies in a hyperplane of dimension less than n. If the trajectory with analytic components does not lie in such a hyperplane then Y_0 will be singular only at isolated points on the trajectory. Denote by $Y^*(t)$ the matrix whose columns are $y^{*\prime}, y^{*\prime\prime}, \ldots, y^{*(n)}$ where y^* is the solution to (7) with $A = Y_0'Y_0^{-1}$, $b = y_0' - Ay_0$, and $y^*(0, y_0) = y_0$. Paralleling the transformations derived for "intrinsic coordinates" in section 2.2 we define an approximate flow by

$$(8) \qquad y^*(t, y_1) = y(t, y_0) + Y^*(t)Y^{*-1}(0)(y_1 - y_0)$$

and we define a transformation to local coordinates by

$$(9) \qquad y(t, y_1) = y(t, y_0) + Y^*(t)Y^{*-1}(0)z(t, y_0, y_1) .$$

At $t = 0$, we will have $z(0, y_0, y_1) = y_1 - y_0$ and z will satisfy the derived system

$$(10) \qquad z' = Y^*(0)Y^{*-1}(t)\{f(y(t, y_0) + Y^*(t)Y^{*-1}(0)z) - f(y(t, y_0))\} - Y^{*'}(0)Y^{*-1}(0)z .$$

It can be checked that if the given dynamical system was of the form

$$(11) \qquad y' = By + c$$

for a constant matrix B and a constant vector c, then the derived equation (10) for z reduces to the trivial system $z' = 0$. It is interesting, therefore, that (9) represents the "general" solution $y(t, y_1)$ of an nth order linear system (11) with constant coefficients as the sum of a particular solution $y(t, y_0)$ through the point y_0 plus the time dependent linear transformation $Y^*(t)Y^{*-1}(0)$ acting on $y_1 - y_0$. The representation will hold if the vectors $y', y'', \ldots, y^{(n)}$ are linearly independent.

We can obtain a more useful version of the transformation with a slight modification by not requiring an exact particular solution $y(t, y_0)$ but rather, since we only really used $y(0, y_0) = y_0$, $y_0', y_0'', \ldots, y_0^{(n)}$, $y_0^{(n+1)}$ we can just as well base the transformation on the approximate particular solution

$$(12) \qquad y^*(t, y_0) = y_0 + y_0't + \ldots + \frac{y_0^{(n+1)}}{(n+1)!}t^{n+1} .$$

We define Y_0, Y_0' just as before and denote by $Y^*(t)$ the matrix whose columns are the successive derivatives of order $1, 2, \ldots, n$ of $y^*(t, y_0)$, namely

$$(13) \quad Y^*(t) = \begin{pmatrix} Y^*_{1j}(t) \\ \vdots \\ Y^*_{nj}(t) \end{pmatrix} = y_0^{(j)} + y_0^{(j+1)}t + \ldots + \frac{y_0^{(n+1)}}{(n+1-j)!}t^{n+1-j}$$

and $Y^{*'}(t)$ is defined just as the derivative of $Y^*(t)$.

Notice we can also write $Y^*(t)$ as

$$Y^*(t) = Y^*(0) + tY^{*'}(0) + \ldots + t^n \frac{Y^{*(n)}}{n!}$$

where the columns of $Y^{*(j)}(0)$ are the derivatives evaluated at $t = 0$ of order $j+1, j+2, \ldots, j+n$ of the approximate particular solution

$$y^*(t, y_0) = y_0 + y_0' t + \ldots + \frac{y_0^{(n+1)}}{(n+1)!} t^{n+1} .$$

The kth column of $Y^{*(j)}(0)$ will be zero if $j + k > n + 1$,

The approximating flow then becomes

$$y^*(t, y_1) = y^*(t, y_0) + Y^*(t) Y^{*-1}(0)(y_1 - y_0) \tag{14}$$

And the transformation to the local z coordinates is

$$y(t, y_1) = y^*(t, y_0) + Y^*(t) Y^{*-1}(0)\, z(t, y_0, y_1) . \tag{15}$$

As before we have $z(0, y_0, y_1) = y_1 - y_0$ and z now satisfies

$$z' = Y^*(0) Y^{*-1}(t)\{f(y^*(t, y_0) + Y^*(t) Y^{*-1}(0)\, z) - y^{*'}(t, y_0)\}$$
$$- Y^{*'}(0)\, Y^{*-1}(0)\, z .$$

We will illustrate the application of the transformation (15) based on an approximating linear system to the system describing the so-called non-linear pendulum

$$y'' + \sin y = 0 \tag{16}$$

or

$$\frac{dy}{dt} = \begin{pmatrix} \frac{dy_1}{dt} \\ \frac{dy_2}{dt} \end{pmatrix} = \begin{pmatrix} y_2 \\ -\sin y_1 \end{pmatrix} = f(y) .$$

We will consider the initial point in the form $y_0 = \begin{pmatrix} 0 \\ \omega \end{pmatrix}$ corresponding to starting the pendulum at the bottom of its swing with angular velocity $\omega \neq 0$. We obtain from (16)

$$y_0' = \begin{pmatrix}\omega\\0\end{pmatrix}; \quad y_0'' = \begin{pmatrix}0\\-\omega\end{pmatrix}; \quad y_0''' = \begin{pmatrix}-\omega\\0\end{pmatrix}.$$

Thus we obtain

$$y^*(t, y_0) = \begin{pmatrix}0\\\omega\end{pmatrix} + \begin{pmatrix}\omega\\0\end{pmatrix}t + \frac{1}{2}\begin{pmatrix}0\\-\omega\end{pmatrix}t^2 + \frac{1}{6}\begin{pmatrix}-\omega\\0\end{pmatrix}t^3$$

$$y^{*\prime}(t, y_0) = \begin{pmatrix}\omega\\0\end{pmatrix} + \begin{pmatrix}0\\-\omega\end{pmatrix}t + \frac{1}{2}\begin{pmatrix}-\omega\\0\end{pmatrix}t^2$$

and

$$Y_0 = \begin{pmatrix}\omega & 0\\0 & -\omega\end{pmatrix}; \quad Y_0' = \begin{pmatrix}0 & -\omega\\-\omega & 0\end{pmatrix}; \quad Y_0'' = \begin{pmatrix}-\omega & 0\\0 & 0\end{pmatrix}$$

and

$$Y^*(t) = \begin{pmatrix}\omega & 0\\0 & -\omega\end{pmatrix} + t\begin{pmatrix}0 & -\omega\\-\omega & 0\end{pmatrix} + \frac{t^2}{2}\begin{pmatrix}-\omega & 0\\0 & 0\end{pmatrix}.$$

We obtain for the transformation to z coordinates

$$y(t, y_1) = \begin{pmatrix}\omega t - \omega t^3/6\\ \omega - \omega t^2/2\end{pmatrix} + \begin{pmatrix}\omega - \omega t^2/2 & -\omega t\\ -\omega t & -\omega\end{pmatrix}\begin{pmatrix}1/\omega & 0\\0 & -1/\omega\end{pmatrix} z(t, y_0, y_1)$$

or

$$y(t, y_1) = \omega\begin{pmatrix}t - t^3/6\\1 - t^2/2\end{pmatrix} + \begin{pmatrix}1 - t^2/2 & t\\-t & 1\end{pmatrix} z(t, y_0, y_1) \tag{17}$$

And $z(0, y_0, y_1) = y_1 - y_0$ while $z(t, y_0, y_1)$ satisfies

$$\frac{dz}{dt} = \frac{1}{1+t^2/2}\begin{pmatrix}1 & -t\\t & 1-t^2/2\end{pmatrix}\begin{pmatrix}0\\\omega t + z_1 - \sin(\omega(t-t^3/6) + (1-t^2/2)z_1 + tz_2)\end{pmatrix}$$

$$\frac{dz_1}{dt} = \frac{t}{1+t^2/2}\left(\sin(\omega(t-t^3/6) + (1-t^2/2)z_1 + tz_2) - \omega t - z_1\right) \tag{18}$$

$$\frac{dz_2}{dt} = \frac{1-t^2/2}{1+t^2/2}\left(\omega t + z_1 - \sin(\omega(t-t^3/6) + (1-t^2/2)z_1 + tz_2)\right)$$

And, in fact, we have the interesting result that

$$(1-t^2/2)\frac{dz_1}{dt} + t\frac{dz_2}{dt} = 0 \quad \text{or} \quad \frac{dz_2}{dz_1} = \frac{t^2/2 - 1}{t} .$$

At each instant t the vector field defined by the differential equation in z coordinates is unidirectional. If these vectors were also of all the same magnitude at a given t then the z flow would carry boxes into boxes by "parallel translation" along the "parallel" trajectory curves. Of course, the magnitude of the vectors is not, in fact, constant so that actually some distortion of z boxes will develop as t increases. We recall that the particular transformation (17) is only intended to be used over the interval in t of one expansion of the z solution (18). At the end of this interval, say at t_1, we evaluate y from (17) and taking $y^*(t_1, y_0)$ as a new y_0 we obtain a new $y^*(t, y_0)$ from (12). Then we get a new Y^* from (13) and a new z transformation from (15) leading to a new (18) which we solve by interval expansion taking the final z box (at $t = t_1$) as the initial z box in the current interval expansion of z. The procedure described in Moore [65] automatically selects the t intervals over which a given expansion is to be used.

3. THE TRANSFORMATION OF E. FEHLBERG

Perhaps the first to consider a problem of the same general type with which we are concerned in this paper was E. Fehlberg [58], who obtained a solution to the following: given a differential equation $y' = f(x, y)$ and assuming one is going to use the Runge-Kutta formula for its numerical solution, is there a transformation $y = y(z, t)$ such that the same numerical procedure applied instead to the derived differential equation for z will lead to improved numerical results in the original variable y?

The similarity between Fehlberg's problem and ours is that they are both special cases of the following very general problem: given a mathematical problem P of type T and a general numerical algorithm A for computing approximate solutions $S(P)$ to all problems of type T, and given a criterion C for comparing numerical solutions with respect to an ordering O, is there a general transformation of variables V such that if P is phrased in a set of variables y, then $V(y)$ defines a new set of variables with respect to which the problem P is transformed into a mathematically equivalent problem, symbolically $V[P]$, also of type T and such that the same algorithm A produces a better (or a best?) numerical solution $S(V[P])$ in the sense of the criterion C? Schematically:

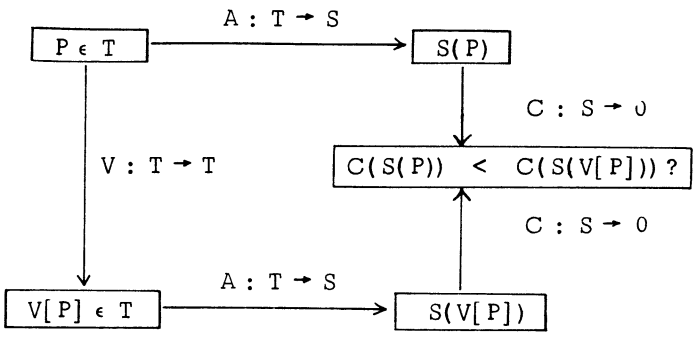

Figure 2

Fehlberg [58], proved the following: the transformation (in a notation close to the original)

$$y = z + y'_0 t + y''_0/2t^2 + (\frac{\partial f}{\partial y})_0 t(z - y_0) \tag{19}$$

leads from $y' = f(t, y)$ to the following derived differential equation for z

$$z' = (1+(\frac{\partial f}{\partial y})_0 t)^{-1}\{f(t, z+y'_0 t + y''_0/2t^2 + (\frac{\partial f}{\partial y})_0 t(z-y_0)) - (y'_0 + y''_0 t + (\frac{\partial f}{\partial y})_0 (z-y_0))\}$$

whose numerical solution by the Runge-Kutta procedure after transformation back to y results in raising the order of the local truncation error by two and also has the property that $(\frac{\partial z'(t,z)}{\partial z})_0 = 0$.

The effect in our case of the transformation (19) will be made clear later when it will appear as a simplification of a deeper and more complicated transformation which we will discuss in section 4 below.

Taken together, a computational algorithm A and a transformation of variables V constitute, in effect, another computational algorithm A'(A, V). This is the point of view taken by Fehlberg in extensions of the above mentioned result, Fehlberg [63, 64], in which he combines, for example, the transformation

$$z = y - \sum_{j=1}^{m+1} \frac{y_0^{(j)}}{j!} t^j$$

for an nth order system $y' = f(t, y)$ with two Runge-Kutta formulas and derives combined transformation-Runge-Kutta algorithms whose local truncation errors are of order $m + 4$ and $m + 5$, respectively.

Various other formulas effectively combining algorithms and transformations have been derived; for example: Pope [63], Dennis [60], Brock and Murray [52], Blanch[52].

4. A LOCAL TRANSFORMATION BASED ON THE CONNECTION MATRIX

During the computation of a numerical solution corresponding to a particular initial point it is not enough to know the behavior of the system just along the particular exact solution. For as soon as any approximation is made and a computed point falls somewhere off the exact solution curve, then we need to know values of the functions occurring in the differential system and, for an error analysis, the behavior of the vector field in a tube surrounding the exact particular solution curve. Even more so, in the problem of the present paper, is the nature of the flow in an entire tube of concern, since this is the very form of our interval vector- or box - valued solutions.

Representing as before, the flow defined by a system $y' = f(y)$, analytic in a region E_n containing an open set about y_0, by $y(t, \overline{y})$, we denote by $C(t, y_0)$ the matrix

$$C(t, y_0) = \frac{\partial y(t, \overline{y})}{\partial \overline{y}} \Big|_{\overline{y} = y_0} ,$$

with components

$$C_{ij}(t, y_0) = \frac{\partial y_i(t, \overline{y})}{\partial \overline{y}_j} \Big|_{\overline{y} = y_0} .$$

We can approximate the flow by

$$y^*(t, y_1) = y(t, y_0) + C(t, y_0)(y_1 - y_0) \tag{20}$$

and y^* will be a good approximation for $\| y_1 - y_0 \|$ small, since for t in a finite closed interval we will have

$$y(t, y_1) = y^*(t, y_1) + O(\| y_1 - y_0 \|^2) . \tag{21}$$

We will call $C(t, y_0)$, the connection matrix for the solution curve $y(t, y_0)$.

Denote the Jacobian matrix of f along a $y(t, y_0)$ by

$$J(t, y_0) = \frac{\partial f(y)}{\partial y} \Big|_{y = y(t, y_0)} .$$

For small enough t and small enough $\|y_1 - y_0\|$ the flow $y(t, y_1)$ will satisfy

$$\frac{\partial}{\partial t}\left(\frac{\partial y(t,\bar{y})}{\partial \bar{y}}\right) = \frac{\partial}{\partial \bar{y}}\left(\frac{\partial y(t,\bar{y})}{\partial t}\right)$$

and we will have

$$\frac{\partial C(t, y_0)}{\partial t} = \frac{\partial}{\partial \bar{y}}\left(\frac{\partial y(t,\bar{y})}{\partial t}\right)\Big|_{\bar{y}=y_0} = \frac{\partial f(y(t,\bar{y}))}{\partial \bar{y}}\Big|_{\bar{y}=y_0} .$$

But

$$\frac{\partial f(y(t,\bar{y}))}{\partial \bar{y}} = J(t, y(t,\bar{y}))\, C(t,\bar{y})$$

so we have

$$\frac{\partial C(t, y_0)}{\partial t} = J(t, y(t, y_0)) C(t, y_0) . \tag{22}$$

Since y_0 is fixed we can shorten the notation to

$$\frac{dC}{dt} = J(t)\, C . \tag{23}$$

From the Taylor expansion

$$y(t,\bar{y}) = \bar{y} + f(\bar{y})\, t + O(t^2) ,$$

we find that at $t = 0$, C is the identity matrix, $C(0) = I$.

Motivated by the approximation y^* given by (20) to the flow $y(t, y_1)$ we define a local transformation of coordinates based on the connection matrix

$$y(t, y_1) = y(t, y_0) + C(t, y_0)\, z(t, y_0, y_1) . \tag{24}$$

Since $C(0, y_0) = I$, we have

$$z(0, y_0, y_1) = y_1 - y_0 . \tag{25}$$

The derived differential system for z (using (23), is

$$z' = C(t)^{-1}\{f(y(t, y_0) + C(t)z) - f(y(t, y_0)) - J(t)C(t)\, z\} . \tag{26}$$

Since $C(t) = I + tJ(0) + O(t^2)$, $C(t)$ will be non-singular for small enough t.

Because of (21), we have

$$z(t, y_0, y_1) = y_1 - y_0 + O(\|y_1 - y_0\|^2) \tag{27}$$

for t in a finite closed interval $[0, T]$ for some $T > 0$.

Thus given a y-box B of width $w(B)$ centered at 0, we will have, for $t \in [0, T]$, the result that the flow in z coordinates satisfies

$$z(t, y_0, y_0 + B) = B + O(w(B))^2 . \tag{28}$$

Therefore for a box B of small width the local transformation (24) is such that in the z coordinates the box tends to remain stationary in time. We will now discuss a computational algorithm based on the transformation (24). We will replace (24) by a more tractable version of the same thing

$$y(t, y_1) = y^*(t, y_0) + C^*(t, y_0) z(t, y_0, y_1) \tag{29}$$

with y^* and C^* chosen to approximate $y(t, y_0)$ and $C(t, y_0)$ by a computationally feasible set of formulas, in a fashion similar to that in section 2.3 above.

4.1 Computation of the connection matrix.

The differential system (22) for C is of order n^2. For $i, j = 1, 2, \ldots, n$, we have

$$\frac{dC_{ij}}{dt} = \sum_{k=1}^{n} J_{ik}(t) C_{kj} .$$

Rather than compute a truncated series expansion for each C_{ij}, we will base our approximating connection C^* on a special form of the solution $C(t)$ to (22) with $C(0) = I$.

We claim that

$$C(t) = \lim_{*} C_n(t)$$

where

$$C_n(t) = \prod_{i=1}^{n} \{I + J(t_{n-i})(t_{n+1-i} - t_{n-i})\} \tag{30}$$

and

$$* = \left(\begin{array}{l} 0 = t_0 < t_1 < t_2 < \ldots < t_n = t \\ \max\limits_{i=1,2,\ldots,n} (t_i - t_{i-1}) \to 0 \text{ as } n \to \infty . \end{array} \right)$$

We have

$$\frac{dC_n(t)}{dt} = J(t_{n-1})C_{n-1}(t_{n-1}) .$$

Therefore as $n \to \infty$ we obtain (22) if $\lim\limits_{*} C_n(t)$ exists. It does, providing t is not too large, for then the Cauchy-Euler polygonal approximations converge. The product (30) is equivalent to application of Euler's method to (22) since

$$C_n(t) = C_{n-1}(t_{n-1}) + J(t_{n-1})C_{n-1}(t_{n-1})(t - t_{n-1})$$

$$= \{I + J(t_{n-1})(t - t_{n-1})\} C_{n-1}(t_{n-1}) .$$

Motivated by the representation (30), we define y^*, C^* as follows. Denote by

$$t_0 = 0 < t_1 < t_2 < \ldots < t_m < \ldots$$

the successive values of t which are going to occur as the places where an expansion of z in Taylor series with interval remainder will be carried out (by the computer, see Introduction above).

Choose a positive integer k (for example, choose $k = d$ for a machine arithmetic equivalent to about d decimal place arithmetic, see Moore [65]), and define $y^*(t, y_0)$ by $y^*(0, y_0) = y_0$ and

$$(31) \qquad y^*(t, y_0) = \sum_{j=0}^{k} \frac{y_{m-1}^{(j)}}{j!} (t - t_{m-1})^j \quad \text{for} \quad t_{m-1} \leq t < t_m$$

and set

$$y_m = \lim_{\substack{t \to t_m \\ t \in [t_{m-1}, t_m)}} y^*(t, y_0) = y^*(t_m^-, y_0) .$$

Define $C^*(t, y_0)$ by

(32) $$C^*(t, y_0) = \{I + J(t_{m-1}, y_{m-1})(t - t_{m-1})\}C^*(t_{m-1}, y_0)$$

or

$$C^*(t, y_0) = \{I + J_{m-1}(t - t_{m-1})\}C^*_{m-1} \quad \text{for } t_{m-1} \leq t \leq t_m .$$

Recall that $C^*(0, y_0) = C^*(t_0, y_0) = I$. The definition is self-consistent since at $t = t_{m-1}$, we have

$$C^*(t_{m-1}, y_0) = (I + 0)C^*(t_{m-1}, y_0) = C^*(t_{m-1}, y_0) .$$

Notice that with the choices indicated by (31) for y^* and by (32) for C^*, the local transformation (29) can be written for $t \in [t_{m-1}, t_m]$ as

$$y(t, y_1) = \sum_{j=0}^{k} \frac{y^{(j)}_{m-1}}{j!}(t - t_{m-1})^j + \{I + J_{m-1}(t - t_{m-1})\} C^*_{m-1} z .$$

Compare this to the transformation (19) of Fehlberg given in section 3 above which we can rewrite for $t \in [t_{m-1}, t_m]$ in the form

$$y(t, y_1) = \sum_{j=0}^{2} \frac{y^{(j)}_{m-1}}{j!}(t - t_{m-1})^j + \{I + J_{m-1}(t - t_{m-1})\} (z - y_{m-1}) .$$

Thus, Fehlberg's transformation (19) appears similar to out transformation (29), putting $k = 2$ in our expression for y^* (eq. 31)), and replacing $C(t, y_0)$ by $I + J_{m-1}(t - t_{m-1})$ in each interval $t \in [t_{m-1}, t_m]$. In virtue of eq. (22), $I + J_{m-1}(t - t_{m-1})$ will be close to $C(t, y_0)$ only for very small t.

4.2 A computational version of the transformation.

Using the definitions (31), (32), we have a computationally feasible local transformation between y and z coordinates of the form given in (29) above.

From (32), we have

$$\frac{dC^*(t, y_0)}{dt} = J_{m-1}C^*_{m-1} \quad \text{in} \quad t_{m-1} \leq t < t_m .$$

The derived differential equation for z is similar to (26), namely:

$$(33)\quad z' = (C^*(t, y_0))^{-1}\{f(y^*(t, y_0)+C^*(t, y_0)z) - y^{*'}(t, y_0) - J_{m-1}C^*_{m-1}z\}$$

in $t_{m-1} \le t < t_m$ and at t_m^- (see eq. (31) above).

From (31), we have

$$y^{*'}(t, y_0) = \sum_{j=1}^{k-1} \frac{y_{m-1}^{(j)}}{(j-1)!}(t - t_{m-1})^{j-1}, \text{ for } t \in [t_{m-1}, t_m^-].$$

This, then, is the system of differential equations which we would submit to our interval expansion program for a Taylor series development (at t_{m-1} about the initial box Z_{m-1}) with interval error bounding. We have already supposed above that the program itself is going to determine t_m, by the procedures described by Moore [65]. Thus for each t in $t_{m-1} \le t \le t_m^-$ a box $Z(t)$ will be defined containing the solutions to (33) through Z_{m-1} and, in particular, the box $Z_m = Z(t_m^-)$ will be computed explicitly, enabling the procedure to be continued to the next interval of expansion $[t_m, t_{m+1}]$.

The only essential matters left unsettled concerning the details of the proposed computational procedure are: (1) the inversion of the matrix $C^*(t, y_0)$ and (2) the computation of the matrix $J = \frac{\partial f(y)}{\partial y}$.

We will take care of the second of these two matters by supposing for now that either a program is provided for evaluating J along with the one for evaluating f by the "user" of our procedure, or else, that a modification of the Taylor coefficient recursion scheme in Moore [65] will enable the computer to compile a program for J, given one for f.

Regarding the inversion of $C^*(t, y_0)$, we note that (from (32))

$$C^*(t, y_0) = \{I + J_{m-1}(t - t_{m-1})\}\, C^*_{m-1} \quad \text{for } t \text{ in } t_{m-1} \le t \le t_m,$$

and therefore

$$(34)\quad \begin{aligned} &\frac{dC^*}{dt}(t, y_0) = J_{m-1}C^*_{m-1} \quad \text{in } t_{m-1} \le t < t_m, \\ &\frac{d^jC^*}{dt^j}(t, y_0) = 0 \qquad (j \ge 2) \end{aligned}$$

in particular

$$C^{*'}_{m-1} = \frac{dC^*}{dt}(t, y_0)\Big|_{t_{m-1}} = J_{m-1} C^*_{m-1} .$$

If we rewrite (33) in the form

$$C^* z' = F = f(y^* + C^* z) - y^{*'} - J_{m-1} C^*_{m-1} z \tag{35}$$

then

$$C^*_{m-1} z^{(j)}_{m-1} + (j-1) C^{*'}_{m-1} z^{(j-1)}_{m-1} = F^{(j-1)}_{m-1}$$

or

$$C^*_{m-1} z^{(j)}_{m-1} = F^{(j-1)}_{m-1} - (j-1) J_{m-1} C^*_{m-1} z^{(j-1)}_{m-1} . \tag{36}$$

Therefore by using (35) we only need to invert C^*_{m-1} in order to carry out the first k terms in the expansion of z at t_{m-1}. Note that the derivatives of $C^*(t, y_0)$ needed in the determination of $F^{(j-1)}_{m-1}$ can be computed easily using (34). For the computation of the remainder term over a region $([t_{m-1}, t_m], B)$ we need to invert the interval matrix

$$C^*([t_{m-1}, t_m], y_0) = \{I + J_{m-1}([t_{m-1}, t_m] - t_{m-1})\} C^*_{m-1}$$
$$= \{I + J_{m-1}[0, t_m - t_{m-1}]\} C^*_{m-1} .$$

We can obtain the required inverse using $(C^*_{m-1})^{-1}$ by carrying out the operations indicated in the expression

$$\{C^*([t_{m-1}, t_m], y_0)\}^{-1} = (C^*_{m-1})^{-1}\{I + J_{m-1}[0, t_m - t_{m-1}]\}^{-1}$$

as an alternative to multiplying the factors first and then inverting.

Replacing t_{m-1} in (36) by the interval argument $[t_{m-1}, t_m]$ and z_{m-1} by a box B we can recursively determine the remainder term for the z expansion by interval computation.

The inversion of the matrices C^*_{m-1} occuring at points of expansion of z can be accomplished with rigorous error bounding by the computer using, for example, a method recently developed by Eldon Hansen, a brief description of which is given in an appendix to this paper. The method is of considerable importance and utility in its own right and will be discussed more fully elsewhere along

with related techniques for other matrix problems such as eigenvalues, eigenvectors, etc.

Since not even the polynomial and matrix computations can be carried out exactly by the computer due to the finite precision of machine arithmetic we are forced to slightly increase the initial z-box, $Z(t_m^+)$ to be used in the interval of expansion $[t_m, t_{m+1}]$ over the final z-box, $Z(t_m^-)$ obtained in $[t_{m-1}, t_m]$. Using interval arithmetic, we compute $Z(t_m^+) = (C_m^*)^{-1}\{(C_m^{*-})Z(t_m^-) + E_m\}$ where C_m^{*-} is a matrix with interval elements obtained by evaluating (32) at $t = t_m$ in interval arithmetic, and C_m^* is a matrix with real elements (machine numbers) obtained by evaluating (32) at $t = t_m$ in ordinary machine arithmetic, and E_m is an interval vector obtained by evaluating $y^*(t_m^-)$, using (31), in interval arithmetic and subtracting the vector, $y^*(t_m^+)$, of mid points of $y^*(t_m^-)$ computed in machine arithmetic. So $E_m = y^*(t_m^-) - y^*(t_m^+)$ and if

$$y^*(t_m^-) = \begin{pmatrix} [a_1, b_1] \\ [a_2, b_2] \\ \cdots \\ [a_n, b_n] \end{pmatrix}, \text{ then } y^*(t_m^+) = \begin{pmatrix} 1/2(a_1 + b_1) \\ 1/2(a_2 + b_2) \\ \cdots \\ 1/2(a_n + b_n) \end{pmatrix}$$

with the averages in $y^*(t_m^+)$ carried out in machine (i.e. non-interval) arithmetic.

An important and delicate question now remains. If the successive t values $t_0 < t_1 < t_2 \ldots < t_m < \ldots$ at which z expansions are carried out get far enough apart then (32) may give too crude an approximation to $C(t, y_0)$ for (29) to do any good in keeping bounds narrow. In this case we could go back to (22) and devise a more accurate approximation to $C(t, y_0)$. However, this would almost certainly complicate the resulting differential system for z; so that somewhere in this direction there is a point of diminishing return.

By reducing the number of terms used in the Taylor expansions, the spacing between successive expansions will decrease (by the computer's choice, based on keeping the local truncation error small), and (32) becomes better. However, at the same time the number of steps to reach a given t value increases and eventually the interval bounds will get wider as $t_i - t_{i-1}$ decreases since we are also keeping track of accumulated round-off error.

The proper balance can perhaps be expressed in terms of a procedure for: (1) choosing the number of terms carried in the y^* series (see eq. (31)), (2) the number of terms to be used in the z series and (3) allowing the successive points of expansion to

depend on an estimate of the error in C^* as well as on the z series remainder.

Computational experience with such a plan will enable various details involved to be fixed in a reasonable manner.

By a straightforward though tedious a priori analysis it can be shown that the transformation (29), as it would be applied by a computer program using the methods described in this section to the example eq. (1), connected with figure 1 in section 1 at successive points $0, \Delta t, 2\Delta t, \ldots, m\Delta t, \ldots$ with $\Delta t < 1$ would lead to a growth in the widths of the bounding interval boxes $Y(\Delta t, y_0), \ldots, Y(m\Delta t, y_0), \ldots$ satisfying

$$w(Y(m\Delta t), y_0)) \leq (1+\Delta t)\, e^{\frac{\Delta t}{2(1-\Delta t)} m\Delta t}\, w(Y(\Delta t, y_0))$$

and therefore the factor of increase per revolution, $m\Delta t = 2\pi$, can be made nearly as small as $(1+(1+\pi)\Delta t)$. Even for Δt as large as $1/4$ the factor should be less than 3.6 per revolution. Compare this with the factor of 500 mentioned in section 1.

A computer program based on the transformation techniques developed in this paper is being prepared for the CDC 3600 at the University of Wisconsin.

4.3 Application of the transformation to Euler's method.

In section 3 above we mentioned that a transformation and an algorithm can be put together into a combined algorithm.

If $z' = g(t, z)$ then Euler's method given z_{m+1} as an approximation to z at t_{m+1} by

$$z_{m+1} = z_m + (t_{m+1} - t_m)\, g(t_m, z_m) \,. \tag{37}$$

Consider the system $y' = f(y)$ and apply Euler's method to the transformed equation (33) using (29). We obtain

$$z_{m+1} = z_m + (t_{m+1} - t_m)\, C_m^{*-1} \{ f(y_m^* + C_m^* z_m) - y_m^{*\prime} - J_m C_m^* z_m \} \tag{38}$$

and

$$y(t_{m+1}, y_1) = y^*(t_{m+1}, y_0) + C_{m+1}^* z_{m+1} \,. \tag{39}$$

Using (32), and (38), we get

$$C^*_{m+1} z_{m+1} = \{I + J_m(t_{m+1} - t_m)\}\{C^*_m z_m + (t_{m+1} - t_m)(f(y^*_m + C^*_m z_m) - y^{*\prime}_m - J_m C^*_m z_m)\} .$$

For example, if $t_m = 0$, $t_{m+1} = t$, $z_0 = y_1 - y_0$ then from (39), (since $C^*_0 = I$ and $y^*_0 = y_0$) we have an approximation to $y(t, y_1)$ of the form

$$Y(t, y_1) = y^*(t, y_0) + (I + J_0 t)\{(y_1 - y_0) + t(f(y_1) - y'_0 - J_0(y_1 - y_0))\}$$

or putting $y^*(t, y_0) = y_0 + tf(y_0)$, we have

$$(40)\quad Y(t, y_1) = y_0 + tf(y_0) + (I + \frac{\partial f}{\partial y}\Big|_0 t)\{y_1 - y_0 + t(f(y_1) - f(y_0) - \frac{\partial f}{\partial y}\Big|_0 (y_1 - y_0))\}.$$

The formula (40) gives an approximation to the solution to $y' = f(y)$ for small t for any initial value y_1 near y_0. Similar formulas can, of course, be derived by combining other algorithms for numerical solution of differential equations with the transformation (29).

5. CONCLUSIONS

We have arrived in section 4 (esp. 4.2) at a transformation procedure with the property sought (28). Roughly, the procedure amounts to carrying along a simultaneous approximate complete set of solutions of the "variational" equations (22), (32), together with an approximate solution $y^*(t, y_0)$ of a particular initial value problem and at the same time using these to define moving coordinates z with respect to which a derived set (33) of differential equations is solved in the transformed variables. This final set (33), is intended to be solved with rigorous automatic error bounding by methods previously developed (Moore [65]). The computations of y^* and C^* do not require error analysis since they are only used to set up a local coordinate system.

Of course, the transformation (29) of interval solutions in z variables back to intervals in y variables must be carried out by interval methods (or in some way with error bounding) in order for the y intervals to be guaranteed to contain the exact solution to a given initial value problem.

The entire computational procedure outlined can be carried out by a computer and constitutes a general scheme for narrowing the width of interval bounds produced by the computer.

The extent to which the scheme is effective in reducing error bounds in practice and the relative cost in computer time of doing this can most easily be determined by actual trials on the computer, and will depend to some extent on the way in which a number of details are arranged.

A useful by-product of the procedure based on the connection matrix in many practical applications is the estimate given by the coefficients of the matrix C^* of the sensitivity of a solution with respect to small changes in initial conditions. Recall that, by definition,

$$C_{ij}(t, y_0) = \frac{\partial y_i(t, y_0)}{\partial (y_0)_j} .$$

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APPENDIX

Abstract of "On Interval Arithmetic in Matrix Computations, Part I"

Eldon Hansen

This abstract is from the first in a series of papers on matrix computations using interval arithmetic to appear in J. S. I. A. M., series B, Numerical Analysis. Only matrix inversion is discussed. However, necessary preliminaries are included for the discussion of determinant evaluation, the solution of linear algebraic equations, and the matrix eigenvalue problem. These topics will be considered in later papers in the series.

Let A^I be a matrix whose elements are interval numbers. We wish to find the set

$$(A^I)^{-1} = \{A^{-1} : A \in A^I, AA^{-1} = I\} .$$

The notation $A \in A^I$ indicates that each element of the (non-interval) matrix A is contained in the corresponding interval element of A^I.

One can attempt to compute $(A^I)^{-1}$ by using an ordinary method for matrix inversion but perform the arithmetic operations in interval arithmetic. It is shown that, for a general interval matrix A^I, such a method suffers from an inherent loss of accuracy.

The method proposed in this paper is longer than such a straightforward approach but, in a sense, minimizes the inherent error. The method is as follows:

Let $A_c \in A^I$. Using ordinary arithmetic, compute an approximate inverse B for A_c. In interval arithmetic, compute A^IB and $(A^IB)^{-1}$. Since $A^IB = I - E^I$ where the interval elements of E^I are "small", it is, in general, possible to express $(A^IB)^{-1}$ in the form $I + E^I + (E^I)^2 + \ldots$. Hence, one can obtain $(A^IB)^{-1}$ by truncating this series (and bounding the resulting error). Alternatively, we can invert A^IB directly in interval arithmetic. As a final step, $(A^I)^{-1}$ is obtained as $B(A^IB)^{-1}$.

As an example, the Hilbert segment of order 3 is represented in interval form as

$$A^I = \begin{bmatrix} 1 & .5 & X \\ .5 & X & .25 \\ X & .25 & .2 \end{bmatrix}$$

where X denotes the interval [.33333 33333, .33333 33334]. Direct inversion in interval arithmetic using infinite precision yields only obout seven correct decimal digits in the computed interval elements of $(A^I)^{-1}$. However, the above method yields about fifteen correct digits.

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