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AUTO: A PROGRAM FOR THE AUTOMATIC BIFURCATION ANALYSIS OF AUTONOMOUS SYSTEMS.

by

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1. Introduction. We describe certain aspects of the recently developed computer program AUTO for the numerical analysis of autonomous systems of the form

$$(1.1) \qquad u'(t) = f(u(t),\lambda), \qquad t \geq 0, \qquad u,f \varepsilon R^n.$$

Here λ is a free parameter. Such systems arise in many areas, especially in the study of chemical reactions, in population dynamics and in mathematical biology. Generally one is interested in both steady state and periodic solutions to (1.1). Since the system contains a free parameter one expects branches of both types of solutions. A steady state bifurcation point is the intersection point of two branches of steady state solutions. A Hopf bifurcation point is the point where a branch of steady states and a branch of periodic solutions intersect. (For background material see for example [3,5,6,8,11,12,15,20].)

Given f, the Jacobian of f, the derivative f_λ, a steady state solution for some value of λ and a number of control parameters, AUTO has the following basic capabilities:

(1) Trace out branches of steady state solutions.

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(2) Accurately locate steady state bifurcation points.

(3) Switch automatically onto bifurcating branches of steady states.

(4) Accurately locate Hopf bifurcation points.

(5) Switch automatically onto branches of periodic solutions and trace out such branches.

(6) Compute past turning points without added difficulty, both on branches of steady state solutions and on branches of periodic solutions.

(7) Compute stable as well as unstable branches. For periodic solutions this is made possible by reformulating the problem as a boundary value problem on $[0,2\pi]$.

(8) Adapt the mesh to the solution. The discretization used is the method of orthogonal collocation with 2,3 or 4 collocation points per mesh interval.

(9) Adaptive stepsize along branches of periodic solutions.

(10) Automatic restarting at certain points.

(11) Store plotting information in files. These files can be investigated by an interactive graphics program.

A more detailed treatment of some of the above mentioned capabilities is given in Section 2. Particular attention is paid to the continuation of branches of periodic solutions. The continuation procedure presented is especially well suited for difficult problems. Examples of the application of AUTO to a representative set of equations is given in Section 3.

Among previous computational work on Hopf bifurcation problems we mention that of [23,24], where a very thorough numerical treatment of a system of two chemical reaction equations is reported. The initial value techniques used there do not generalize to systems of dimension greater than two, when unstable branches of periodic solutions are to be computed. Extensive numerical computations on the Hodgkin-Huxley model are given in [18]. See also [22]. Also included in [18] is the computation of branches resulting from period doubling bifurcations. In AUTO this added capability is intended to be implemented also. Computational aspects of the Hopf bifurcation problem are also considered in [16], where projection methods are used.

2. The Continuation of Periodic Solutions. The computation of branches of steady state solutions is an algebraic problem. It consists of the bifurcation analysis of the equation

$$f(u,\lambda) = \emptyset.$$

This can be accomplished numerically using the arclength-continuation and branch switching techniques of [9]. (See also [17].) The techniques of [9] apply in a very general setting. In fact the continuation of periodic solutions can be treated in the same framework.

First we recall the basic features of the general procedure in [9]: Consider the operator equation

$$G(u,\lambda) = \emptyset, \tag{2.1}$$

where λ is a parameter and G a nonlinear mapping from one Hilbert space into another. Let $w \equiv (u,\lambda)$. If there exists some parametrized branch $w(s)$ of solutions to (2.1) then under appropriate smoothness assumptions we have

$$G'(w(s))\, w'(s) = \emptyset.$$

Thus the derivative G' always has a nullspace along the branch. Assume now that we have a solution $w_\emptyset$ of (2.1), i.e. $G(w_\emptyset)=\emptyset$, and that in addition the nullspace of $G'(w_\emptyset)$ is spanned by a vector $w_\emptyset'$. Thus the nullspace is one dimensional. Let $w_\emptyset'^*$ be the adjoint element such that $w_\emptyset'^* w_\emptyset' = 1$. Then the inflated problem

$$G(w) = \emptyset$$

(2.2)

$$w_\emptyset'^*(w-w_\emptyset) - s = \emptyset,$$

which we write more compactly as

$$H(w,s) = \emptyset,$$

has the solution $w=w_\emptyset$ when $s = \emptyset$. Further the derivative

$$H_w(w_\emptyset,\emptyset) = \begin{pmatrix} G'(w_\emptyset) \\ w_\emptyset'^* \end{pmatrix},$$

is clearly nonsingular. Hence the implicit mapping theorem guarantees the existence of a branch of solutions $w(s)$ for small s.

Numerical techniques can be based directly on (2.2). If $G(w) = \emptyset$ represents a differential equation, then of course the equation must be discretized first. Further for numerical purposes it is often more convenient to use the approximation $w_\emptyset' \simeq (w(s)-w_\emptyset)/s$. If in addition we solve (2.2) for only one value of s, say $s=\Delta s$, then (2.2) becomes

$$G(w) = \emptyset$$

(2.3)

$$(w-w_\emptyset)^*(w-w_\emptyset)/\Delta s-\Delta s = \emptyset.$$

Essentially the same procedure can be used to switch branches at a bifurcation point after the direction of the bifurcating branch has been computed. In this situation one replaces $w_\emptyset'$ in (2.2) by such a direction.

The general procedure of [9] outlined above has been applied by various authors. See for example [2,4,7,1Ø,13,21].

Now consider the problem of determining branches of periodic solutions to the autonomous system (1.1). First note that not only the periodic solution u, but also its period ρ changes along such a branch. To fix the period, linearly map $[\emptyset,\rho]$ into $[\emptyset,2\pi]$. This transforms the differential equation into

$$u'(t) = \frac{\rho}{2\pi} f(u,\lambda), \tag{2.4}$$

where the unknown period ρ now appears explicitly and where 2π-periodic solutions are to be determined, that is, we impose the condition

$$u(\emptyset) = u(2\pi). \tag{2.5}$$

This effectively replaces the original problem by a boundary value problem with non-separated boundary conditions. In particular this makes the computation of asymptotically unstable solutions possible. Unstable and therefore unphysical solutions frequently must be computed in order to reach stable solutions elsewhere on the branch.

Suppose $(\lambda_0, \rho_0, u_0(t))$ defines a known periodic solution of (2.4), (2.5). The objective is to set up the equations for finding a solution nearby on the branch. A remaining difficulty is the inherent non-uniqueness of u, due to the fact that a periodic solution can be translated freely in time. For numerical computation the new solution u must be "anchored". There are many possible choices for an additional equation to accomplish this. One is to simply fix one of the components of u at $t=0$. However the resulting set of equations has an isolated solution only under conditions that are not required for the underlying problem itself. For theoretical purposes a better choice is the orthogonality condition

$$(2.6) \qquad (u(0) - u_0(0))^T f(u_0(0),\lambda) = 0,$$

which ensures that $u(0)$ on the orbit to be determined occupies a similar position as $u_0(0)$ on the known orbit. Indeed continuation proofs can be based on the equations (2.4)-(2.6). Below it will be shown, however, that an integrated version of (2.6) is more appropriate for practical numerical computation.

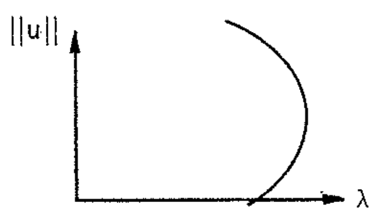
The equations (2.4)-(2.6) can be viewed as being of the form (2.1), that is, they can be written as $G(w) = 0$, with $w = (\lambda,\rho,u)$. Thus from the general case it follows that we must add the continuation equation

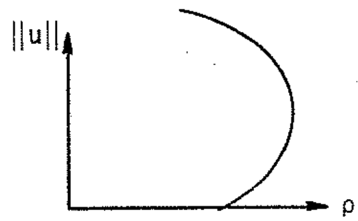
$$(w-w_0)^*(w-w_0)/\Delta s - \Delta s = 0,$$

which in this application can be written as

$$(2.7) \qquad c_1^2(\lambda-\lambda_\emptyset)^2/\Delta s + c_2^2(\rho-\rho_\emptyset)^2/\Delta s$$
$$+ c_3^2\int_\emptyset^{2\pi} (u-u_\emptyset)^T (u-u_\emptyset)/\Delta s \, dt - \Delta s = \emptyset .$$

Here the constant weights c_i, $i=1,2,3$, are included for generality. The equations (2.4)-(2.7) can be used without modification when turning points are present on a branch of periodic solutions, that is, when either of the situations in the diagrams below is encountered:





Indeed the capability to compute past turning points is the main advantage of using the inflated system (2.3).

To illustrate the performance of the computational scheme (2.4)-(2.7) consider the simple problem

$$(2.8) \qquad \begin{aligned} u_1' &= (1-\lambda)u_1 - u_2 \\ u_2' &= u_1 + u_1^2 . \end{aligned}$$

For all λ the steady state $u_1 = u_2 = \emptyset$ is a solution. The Jacobian of the right hand side of (2.8) has a conjugate pair of eigenvalues cross the imaginary axis when $\lambda = 1$, signalling a Hopf bifurcation point. The bifurcating branch of periodic solutions is in this example a vertical line-segment. (See Figure 1.) The branch of periodic solutions does not extend to infinity however, as it would have done for the linear problem without the u_1^2 term. In fact the branch has a limit point. When approaching this limit point the phase cycles tend to a separatrix, while the period goes to infinity. This behaviour is displayed in the phase diagram of Figure 2. The labels in Figure 2 correspond to those in Figure 1. Figure 3 shows the second solution component as a function of time. Note that along the branch the maximum value of u_1 is attained at different values of the independent variable t. In other words the peaks move as we go along the branch of periodic solutions. What is worse, this motion becomes more pronounced as the fronts get steeper. Such a property is very undesirable. For if u has rapidly changing components, then an adaptive mesh will be necessary. What may be a good mesh for a given solution point on a branch of periodic solutions, may not be good at all for a solution point nearby on the branch, if steep peaks are subject to translation. The result will be that the equations (2.4)-(2.7) require a very small stepsize Δs along the branch. Of course this unwanted property is not inherent in the problem to be solved, but rather it is due to the anchor equation (2.6).

To derive an alternative for (2.6) that performs better on difficult problems, assume again that $(\lambda_\emptyset, \rho_\emptyset, u_\emptyset)$ represents the known solution and that a neighbouring solution (λ, ρ, u) is to be determined. If $u(t) = v(t)$ is a solution then so is $v(t+r)$ for any r. It is natural among this infinity of solutions to seek the one that minimizes the distance

$$(2.9) \qquad \int_\emptyset^{2\pi} (v(t+r) - u_\emptyset(t))^2 \, dt$$

over r. In the example this would force the peaks to remain approximately in the same place. The minimizing

r^* is obtained by setting the derivative of (2.9) with respect to r equal to zero:

$$\int_0^{2\pi} (v(t+r^*) - u_0(t))v'(t+r^*)\,dt = 0 .$$

Letting $u(t) = v(t+r^*)$ and approximating $u'(t)$ by $u_0'(t)$ we obtain

$$(2.6)^* \qquad \int_0^{2\pi} (u(t) - u_0(t))u_0'(t)\,dt = 0.$$

Note that $(2.6)^*$ is nothing but an integrated version of (2.6). Also recall that while $(2.6)^*$ requires the distance between u and u_0 to be minimized, there is also equation (2.7) which essentially requires the distance between (λ_0, ρ_0, u_0) and (λ, ρ, u) to be equal to Δs.

Recomputing the bifurcation problem corresponding to equation (2.8), but with $(2.6)^*$ replacing (2.6), we obtain Figure 4 corresponding to the old Figure 3. The results clearly show the advantage of using the modified anchor equation $(2.6)^*$. A complete argument to verify that use of $(2.6)^*$ leads to a well-posed problem is not difficult.

3. Numerical Examples. In this section we present the results of applying AUTO to a number of examples. These results are given in the form of bifurcation diagrams and accompanying phase diagrams. Labels with accompanying dashed line segments (----) in the bifurcation diagrams denote solution points for which plotting information has been stored. The frequency of storing plotting information is user controlled. Also user specified are the limits of the bifurcation diagram as well as the maximum number of steps along any branch. For periodic solutions the number of meshpoints NTST is fixed and selected by the user. Their distribution can be made to adapt automatically to

the solution during computation along a branch. In the bifurcation diagram NCOL denotes the number of collocation points per mesh interval. The mesh selection algorithm used is basically that of [19]. In fact the collocation method employed can be viewed as a subset of COLSYS [1] for the numerical solution of the special class of problems considered in this paper. Such specialization should result in a more efficient code. Computation time and storage are important considerations in AUTO, because in any given run the system of autonomous equations may have to be solved hundreds of times.

Example 3.1 The system considered is

$$u_1' = \lambda \sin(u_1) - u_2$$
$$u_2' = 2u_1 - u_2,$$

which has the steady state solution $u_1 = u_2 = 0$ for all λ. A Hopf bifurcation from the zero solution takes place at $\lambda=1$ and a steady state bifurcation at $\lambda=2$. Two other Hopf bifurcation points are located on the secondary branch of steady states. (See Figure 5 and the local enlargements in Figures 6 and 7. Branches 1 and 2 in Figure 5 are steady states, while branches 3, 4 and 5 represent periodic solutions.) Disregarding other possible solutions not displayed in Figure 5, we note that for λ in $[0,1]$ there is only the zero solution. When λ becomes greater than 1, a limit cycle forms around the zero steady state. When λ passes the vale 2, two new solutions branch off from the zero steady state. When λ passes the value 2.54, limit cycles appear around these new steady states also. As λ approaches the value 2.70 these limit cycles grow and each approaches a separatrix, whereby the period goes to infinity. Simultaneously the outer large limit cycle contracts and approaches the union of the limiting configurations of the two smaller limit cycles. The situation is illustrated graphically in Figure 8.

Example 3.2 A three dimensional example is

$$u_1' = (1-\lambda)\sin(u_1) - \sin(u_2) - u_3^3$$

$$u_2' = (2-\lambda)\sin(u_1) + u_2^2$$

$$u_3' = \sin(u_3) + u_2^2 - u_1^2 .$$

The bifurcation diagram generated by AUTO is given in Figures 9 and 10. (Branches 1 and 2 in Figure 9 are steady states, while 3 and 4 represent periodic solutions.) There is one steady state bifurcation point and there are three Hopf bifurcation points. The branch of periodic solutions (3) bifurcating from the zero steady state branch (1) at $\lambda=1$, reattaches itself to the nontrivial steady state branch (2) at $\lambda=1.88$. The projection of some limit cycles along this branch onto the u1,u3-plane are given in Figure 11. The second periodic branch (4) in the diagram does not reattach itself to any steady state branch.

Finally consider a physically more realistic example. For previous computations see [23,24].

Example 3.3 The dynamic behaviour of a single first order chemical reaction in a continuously stirred tank reactor can be modelled by the ordinary differential equation

$$u_1' = -u_1 \;\; +B\ Da\ (1-u_2)\exp(u_1) - \beta u_1$$

$$u_2' = -u_2 + Da\ (1-u_2)\exp(u_1),$$

where B,β and Da are dimensionless parameters. For β=3 and B=14 the bifurcation diagram is given in Figure 12. There are two Hopf bifurcation points. Figure 13 displays the second solution component versus time along the branch of periodic solutions.

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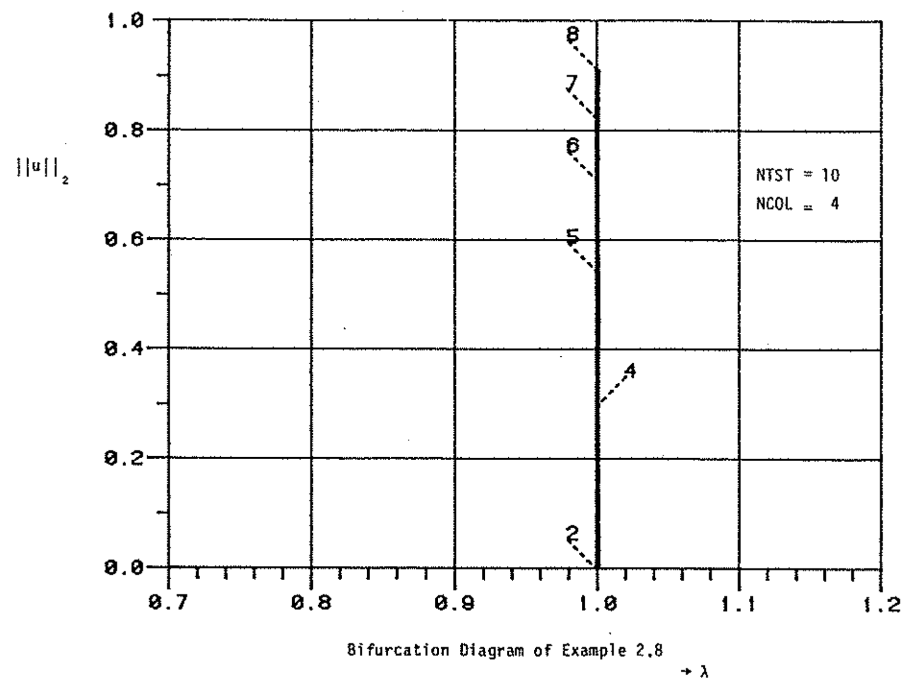
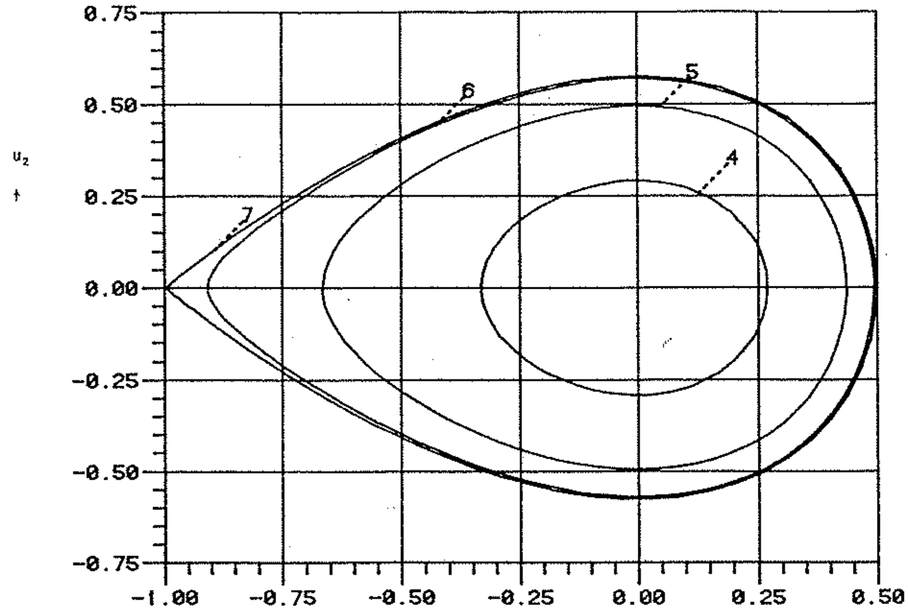


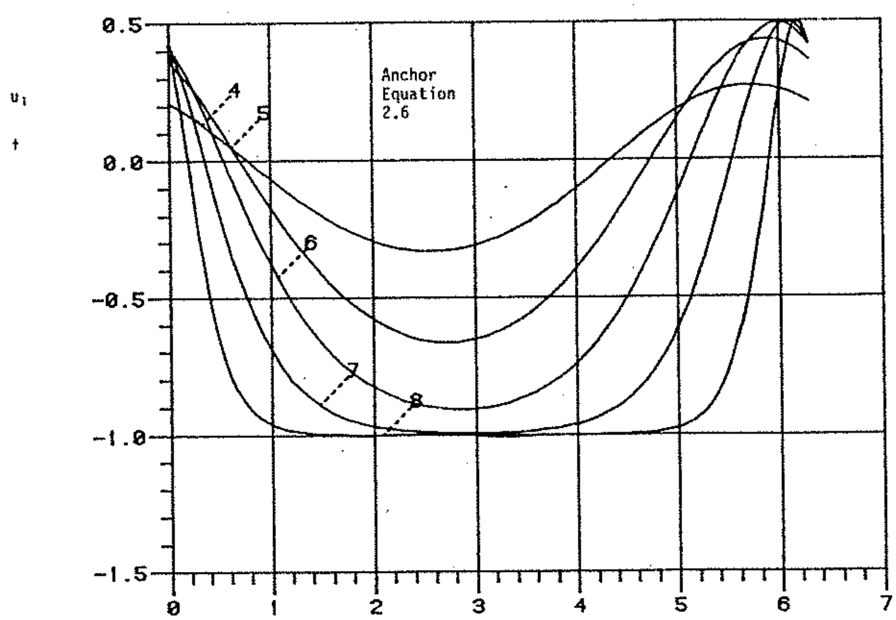
Bifurcation Diagram of Example 2.8

FIGURE 1



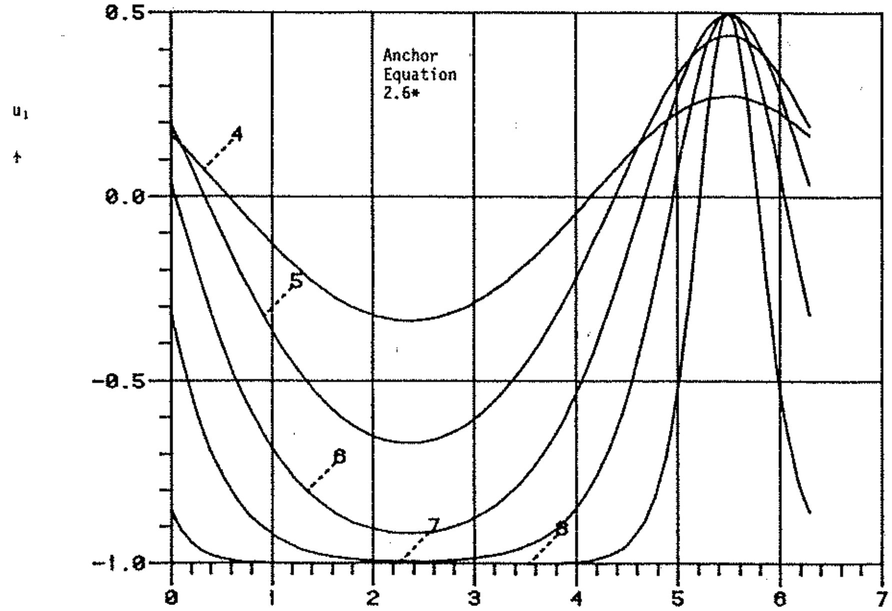
Phase-Plane Curves of Example 2.8 $\to u_1$

FIGURE 2



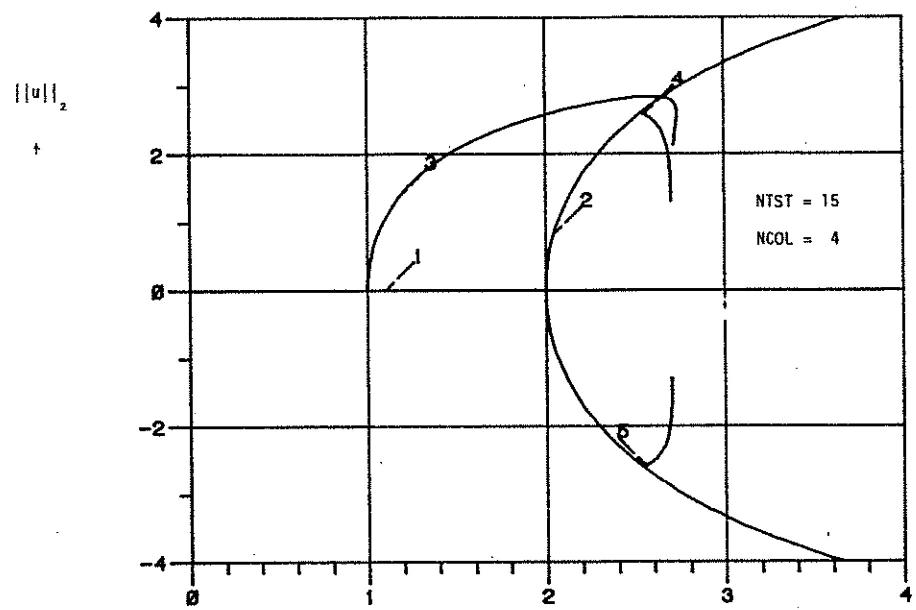
First Solution Component along the
Branch of Periodic Solutions in Example 2.8 $\to t$
[Using Anchor Equation 2.6]

FIGURE 3



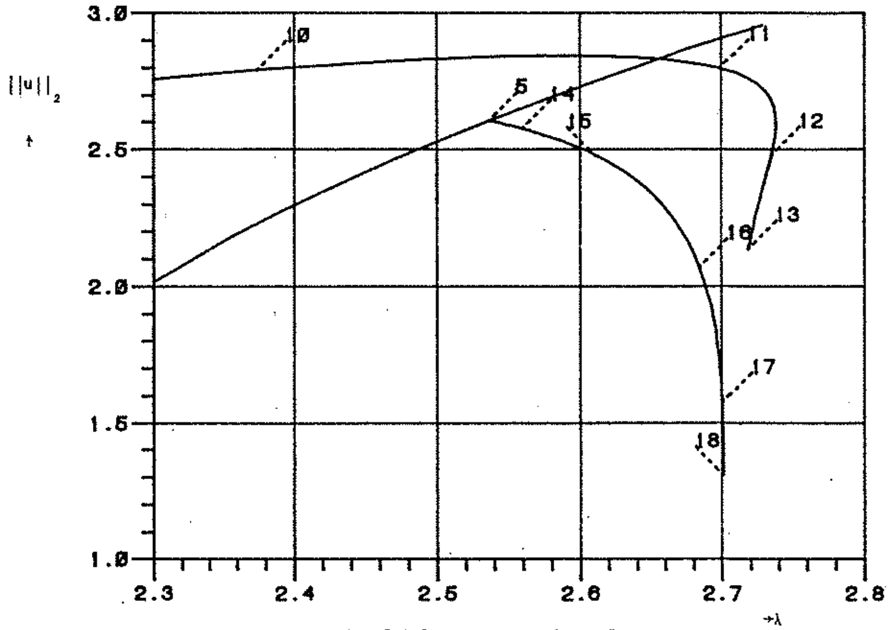
First Solution Component along the
Branch of Periodic Solutions in Example 2.8
[Using Anchor Equation 2.6*.]

FIGURE 4



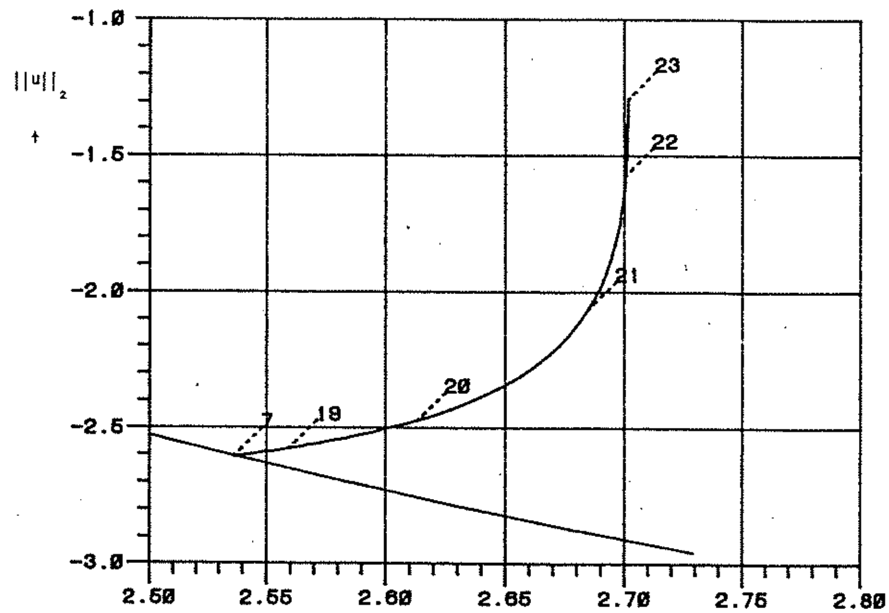
Bifurcation Diagram of Example 3.1

FIGURE 5



Local Enlargement of Figure 5

FIGURE 6



Local Enlargement of Figure 5

FIGURE 7

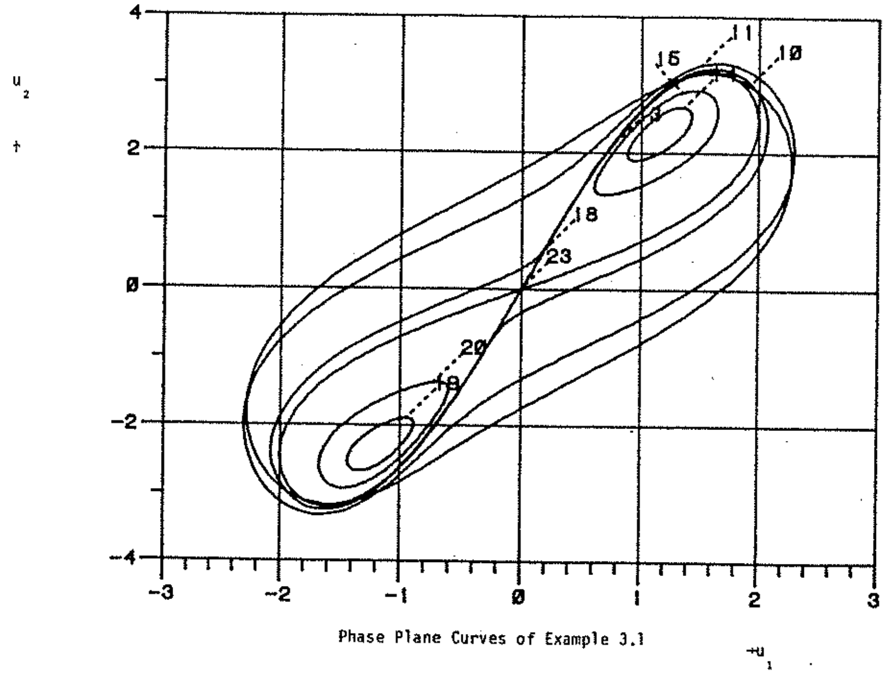


FIGURE 8

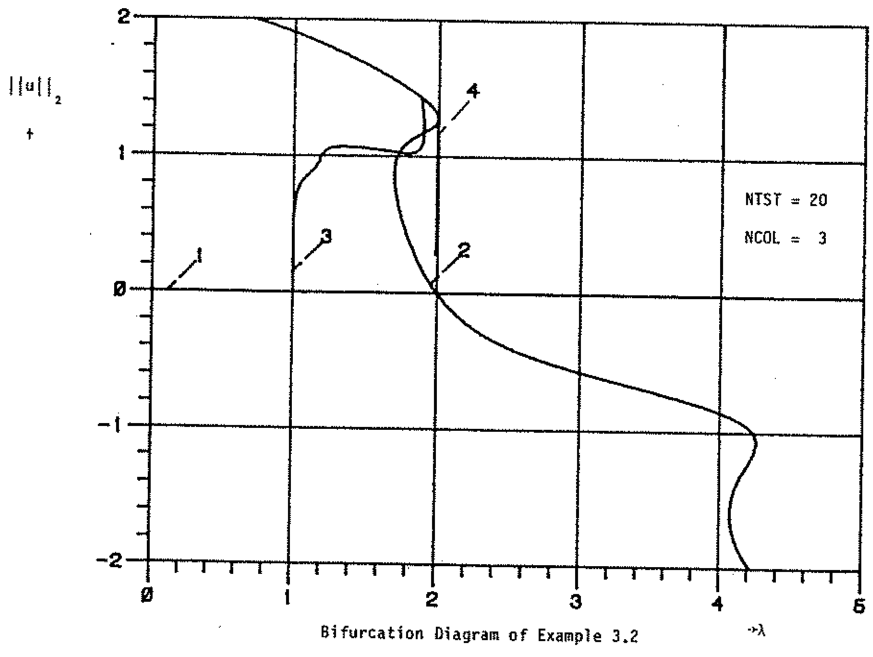
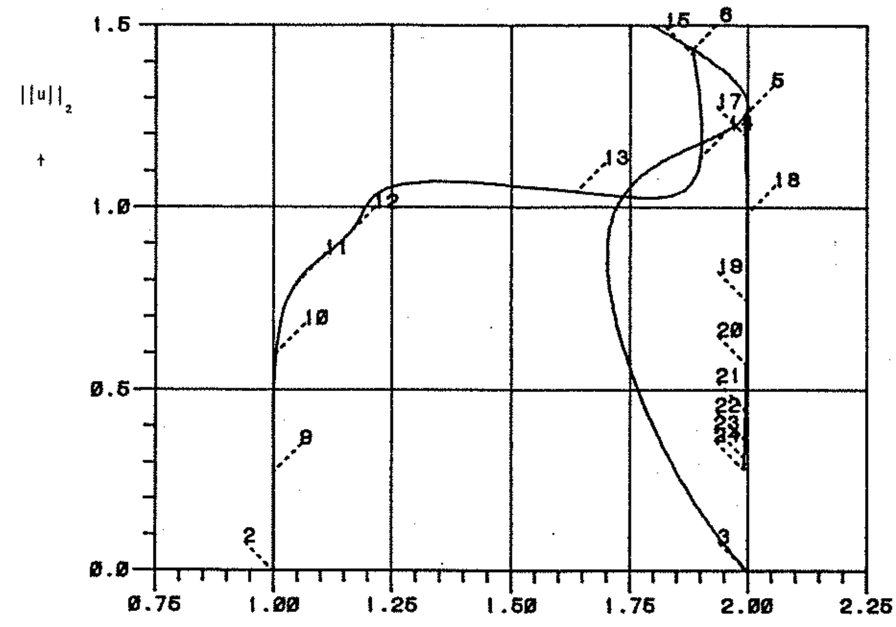
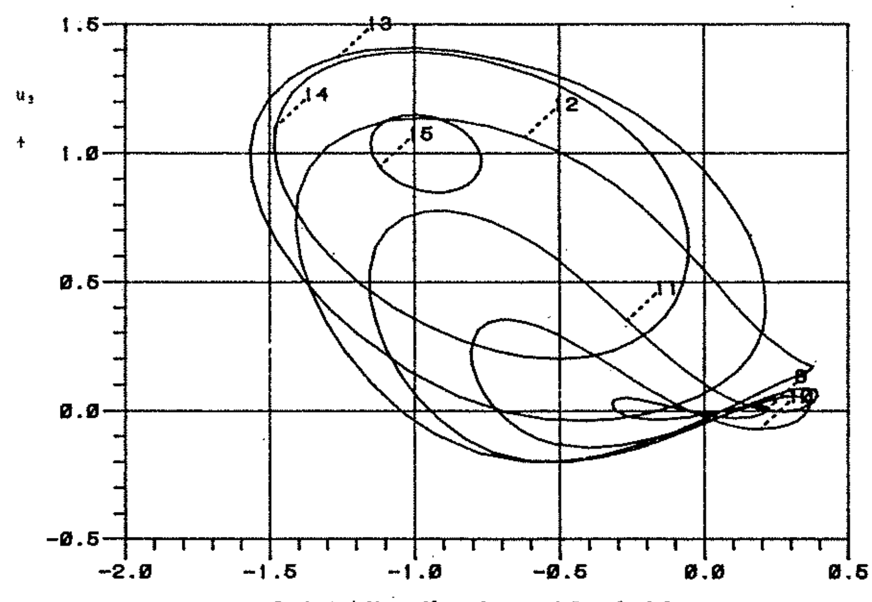


FIGURE 9



Local Enlargement of Figure 9

FIGURE 10



Projected Phase-Plane Curves of Example 3.2

FIGURE 11

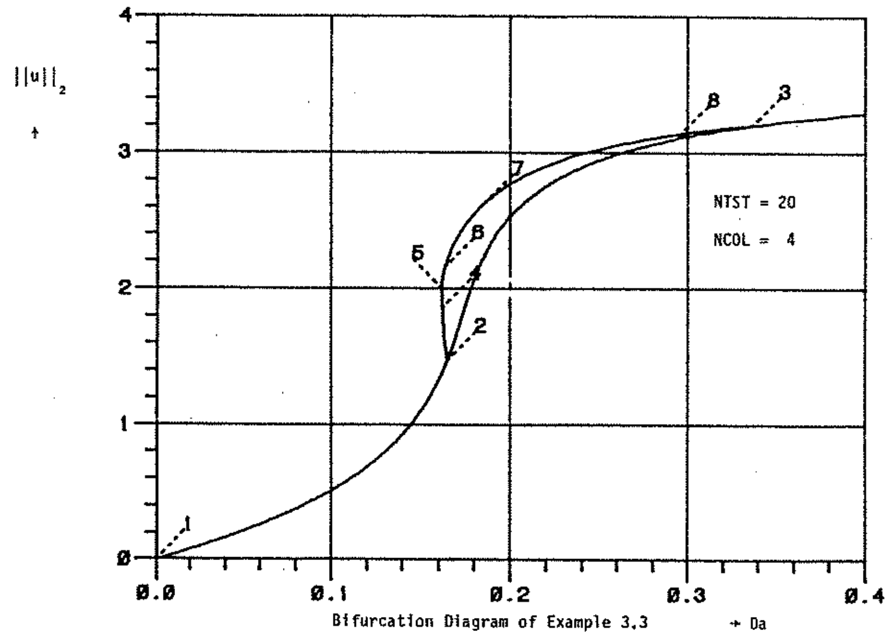


FIGURE 12

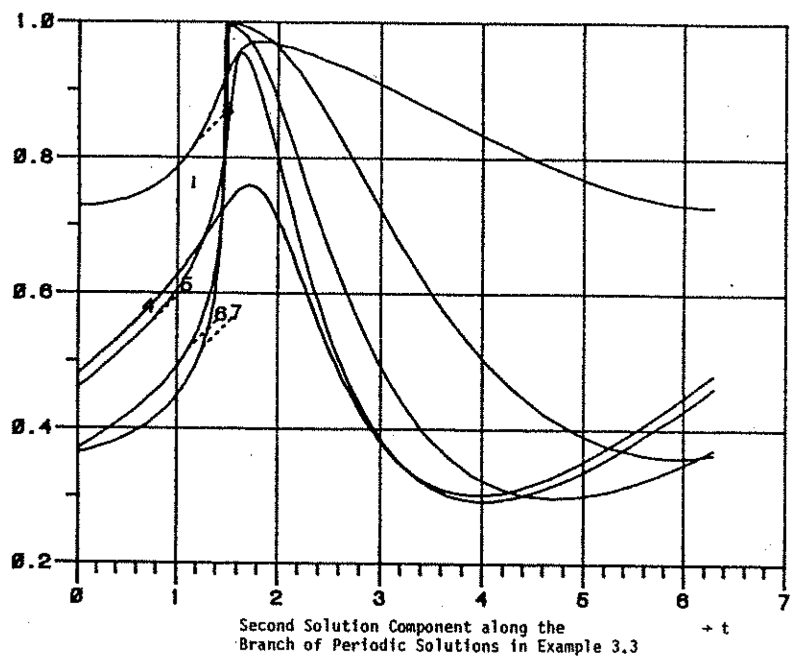


FIGURE 13

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