INTERNATIONAL INSTITUTE FOR IASA APPLIED SYSTEMS ANALYSIS CONFERENCE PROCEEDINGS

ANALYSIS AND COMPUTATION OF EQUILIBRIA AND REGIONS OF STABILITY

With Applications in Chemistry, Climatology, Ecology, and Economics

RECORD OF A WORKSHOP

July 21 — August 1, 1975

H. R. Grümm, Editor

SCHLOSS LAXENBURG A-2361 AUSTRIA

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The views expressed are those of the contributors and not necessarily those of the Institute.

The Institute assumes full responsibility for minor editorial changes made in grammar, syntax, or wording, and trusts that these modifications have not abused the sense of the writers' ideas.

Preface

This record has been put together in a limited time for prompt distribution. It is not a proceedings volume. Rather it is a collection of all memoranda, diagrams, and literature references that were circulated before the workshop, used to support presentations during the workshop, or written down to preserve some ideas and some outcomes of computations that arose from the workshop. The only organizing principle is the temporal sequence in which the materials were presented or prepared.

T.C.K.

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Advance Description of Workshop

In the last few years problems have come to the fore in Climatology, in ecology, and in economics that have a common mathematical structure.

In climatology and ecology, these problems concern systems described by a set of differential equations in which non-linearities are an important aspect of the problem. Mathematical treatment has therefore emphasized simplifying assumptions or complex simulations. The former destroys many subtle behavior characteristics while the latter can be expensive, and may lack the generality needed for transfer of findings to other situations.

Another handhold for analysis is present if the system has the property that as time proceeds the motion of the state variables approaches an asymptote (or rest point). Mathematically, such a rest point also qualifies as a stationary solution of the differential equations. Moreover, such a solution can also be considered as a fixed point of a continuous mapping of the set of possible initial states into itself.

In the economic theory the notion of a fixed point is the principal mathematical tool for the analysis of economic equilibria. However, unlike in the other two fields, the representation of the path to equilibrium has not received comparabel emphasis in the research in economics of the last decade.

In all three fields there is a need for methods to find the fixed points or rest points of the system if such exist, and also for each such point the "basin" (or region of stability),

that is, the set of initial conditions from which the solution ultimately approaches a given fixed point. The ecological concept of resilience is closely related to the notion of the basin.

As to the computation of fixed points, the methods most in use by the climatologists depend on tracing a path from a suitable initial state through time until it stabilizes. For analyzing the sensitivity of climate to specified present or possible future effects of man's activity such a calculation has been made for both the unperturbed ("base-line") equilibrium and fro the perturbed alternative. G.I. Marchuk has developed a procedure that replaces the second calculation by an approximation utilizing the result of the first and exploiting the bilinearity of the equations. One should ask further whether, if knowledge of the equilibrium without the details of the path has value in itself, one could also dispense with the first calculation, using methods and algorithms to approximate the unperturbed and perturbed equilibria directly.

Among the methods that should be explored and tried out on moderate-size examples are any one or possible combinations of

- (a) Direct solution of some finite-difference approximation to the differential equations defining a steady state,
- (b) Fixed point algorithms such as have been developed in economics in the last 6 years (Scarf, Hansen, Kuhn, and others),

- (c) Extrapolation procedures such as those developed by Aitken, Shanks, and others,
- (d) Gradient methods and, in particular, Newton or quasi-Newton methods.

Of these, (a), (b), (d) need supplementation by a procedure to ascertain the stability properties of the equilibrium or equilibria found.

In other cases, in any of the three fields, the ultimate nature of a solution of the system of differential equations may be not an approach to a single limit point, but an approach to a limit cycle, or to another less regular path that remains within an "attractor set" of dimensionality much less than that of the space of state variables. It is desirable to explore the possiblity of generalizing the methods found suitable for limit points to the determination of limit cycles if that case pertains, or else to the placing of bounds on the attractor sets, or the estimation of means and variances of indefinitely continuing motion.

The study of any of these several problems should, in an institute for applied systems analysis, be accompanied by tryouts of calculations on models from the three fields that in the beginning have a rather small number of dimensions, to be followed later by more ambitious tests if the results are encouraging.

In particular, in regard to climatology, the proposed tryout problems might include prototype problems of the effects on climate of large and sustained waste heat releases in various

locations, such as have been made by and for the IIASA Energy
Project. A valuable focus for ecological tryouts is the Ecology
Project's present Pacific salmon fishery management study, with
a spectrum of six to eight models of growing complexity. Economic
examples would be brought in by participants.

To stimulate research along the lines described, we are holding a two-week summer workshop at IIASA, July 21 through August 1, 1975. We are inviting about three people each from climatology, ecology, and economics whose main concern is that the models are, within chosen limitations of size and complexity, good representations of significant real phenomena. In addition, we are inviting four or five people who are specialists in algorithm development and tryout. This adds up to about 15 invited scientists minus some allowance for people who belong in more than one category. About six to ten IIASA staff members would take regular part in the work of the workshop. One or two computer programmers should also be allowed for.

We have in mind an intensive working group which pretty much writes its own ticket with regard to frequency of discussions and formation of subgroups, except that a few plenary overview sessions are to be scheduled at the beginning and at the end.

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OPENING PLENARY SESSION, SCHLOSS, JULY 21, AM

Welcoming Remarks to the Participants

<u>Koopmans</u>: Dr. Roger Levien has agreed to make a few welcoming remarks on behalf of IIASA. Dr. Levien is slated to succeed Professor Raiffa as Director of IIASA this fall.

<u>Levien</u>: Thank you. IIASA is a complex dynamic system, and its establishment was part of a conscious policy intended to encourage equilibrium and stability in the world system. Whether that policy will succeed or fail, it is too early to determine. All we can say is that so far the local conditions are good.

In the spirit of science I want to describe the behavior of this dynamic system, IIASA, beginning with its initial conditions. Those occurred at the end of 1966 when President Johnson of the United States asked his former National Security Advisor, McGeorge Bundy, to explore the possibility of establishing, jointly with the Soviet Union, a center for research on problems common to developed countries. Bundy travelled to Moscow where he met Professor Jerman Gvishiani, the Deputy Chairman of the State Committee of Science and Technology. After initial discussions it was decided that the idea warranted further exploration.

A series of negotiations then took place from 1967 through 1972 and proceeded in ever widening circles, engaging more and more countries in the discussion. By October 1972 when the negotiations culminated in the signing of the charter at the Royal Society in London, there were twelve member organizations

who subscribed to the charter. What they subscribed to was a charter creating an institution that was non-governmental, independent, and of scientific character, to work on those problems that arise as a result of scientific and technological progress-the general difficulties facing the world today. The countries represented were the US and the USSR, by their Academies of Sciences; and the UK, France, Poland, CSSR, FRG, GDR, Italy, Bulgaria, Japan, and Canada, by analogous organizations—in some cases, a specially created scientific institution such as the Committee on Applied Systems Analysis of Canada. An important characteristic of these founding members is that they are non-governmental scientific organizations.

The twelve organizations committed themselves to budget contributions which fell into one of two categories: each of the category A members--the US and USSR--contributes one million US dollars a year, and each of the category B members 150,000 US dollars. The initial contributions were thus on an annual basis of 3.5 million dollars. In 1973 Austria became a member through its Academy of Sciences, and in 1974 Hungary joined, so that there are now fourteen national member organizations and budget contributions of 3.8 million US dollars. In this one regard the founders showed less than perfect foresight, because they established the contribution schedule in terms of US dollars. At that time it was unclear where IIASA was going to be located-whether in France or in Austria, the two contenders -- so the dollar was chosen as the common denominator. But shortly after the charter was signed the dollar was devalued and has been several times since; and of course inflation has cut into the real value of the contributions. Less actual money is available for the institute than had been intended. Nevertheless, our

growth has been satisfactory, and as you can see, we are now located in Austria in this marvelous Schloss, which has been donated by the Austrian government and renovated with their funds.

The Central Court was completed in December of 1974, and I think this is a good point to use to characterize the initial trajectory. I told you something about the initial conditions. Work started here in May 1973, when one scientist, one project and one corridor of the Schloss were ready to go. In fact at that time Howard Raiffa used to take visitors around, open the door of the one scientist's office, and say: "And here is a typical IIASA scientist at work." Well, that typical scientist has grown from one in May 1973 to in the order of 70 right now. The one project has grown into eleven, and the one corridor into most of the Schloss. Over the next years the Austrian government will be renovating the remainder of the Schloss that you can see when you walk outside.

Now let me say something briefly about the current state of the Institute. There are eleven projects, as I mentioned. I find it convenient to group them into a few categories. We have an area that you might call the resources and environment area. Here three projects are actively under way. One of them, in the water resources area, has been primarily concerned with the management of river basins, looking at a couple of examples: the Vistula River and the Tisza River, both in Eastern Europe. The ecology project has been concerned with the management of complex ecological systems. We will hear more about their work today, but I might mention quickly that their approach has been

a detailed examination of actual examples. They began with extremely interesting work on the managment of a forest pest, the spruce budworm, which is endemic in Eastern Canada but also in Poland, the USSR, Japan, and the US. The project did work on the complex policies involved in controlling this dynamic system. Then they investigated international fishery, that of the Pacific salmon which is exploited by four different countries: Canada, the US, Japan, and the USSR. They have also studied the Obergurgl region of Austra, to look at the impact on a rather fragile Alpine ecosystem when its natural resources are exploited for tourism.

The third project, just beginning now, will concern itself with world's food and agricultural problems. I can't say too much yet about what we'll do, except that like many other people we are aware that these are central problems of the future, and we ought to have a bare understanding of their dynamics, the potential, the way in which maximum exploitation in value can be obtained from our few resources.

The next grouping of activities concerns human settlements and social services. Here we have a project on urban and regional development which has been focused primarily on national settlement systems; that is, the ways in which people are located around countries and the dynamics which govern demography and mobility in various kinds of societies—those which are centrally planned, those which are market societies, and so on. Of course, we are taking advantage of the opportunity that IIASA represents to compare alternative policies and different kinds of societies. We have also been looking at municipal management, and the

question of managing urban emergency services and urban traffic problems. The second project under the heading of human settlements and services is the bio-medical project, and here again we are really just beginning to build up momentum. Our concern is with two issues--modelling national health care systems, in particular trying to compare their structure in different kinds of economies; and coordinating international bio-medical research programs, on which we will be cooperating with WHO.

A third category is a management and technology grouping; here we have two projects. The one on large organizations has again taken the opportunity to do comparison studies. Last year we looked carefully in a retrospective way at the management of a complex regional development system, the Tennessee Valley Authority in the US. We held a very large conference last November/December on the TVA, with a heavy representation from the TVA, and from the USSR and other member countries, to discuss the techniques used in developing that forty-year-old system and in managing it. But what makes that particular instance interesting is that at the end of the year we will have a comparable case study on the Bratsk-Ilim development in Siberia. So we will be able to compare carefully the ways in which large regional developments based on hydro-power have progressed in both the US and the USSR. And we hope to follow that up with yet another such comparison, either in a developing country or in Japan.

We have an integrated industrial systems project which has been doing another kind of comparison: an around-the-world

comparison of the way in which the steel industry is managed, with a focus on production planning, from very long-term to day-to-day planning. This comparison has involved examination of the steel industry in Japan, the USSR, the FRG, the CSSR, the US, the UK, and so on. The result has been a distillation of the world state of the art and an appreciation of what advances are likely to occur in the management of the steel industry.

A little closer to home, we have a fourth grouping which I would say is the scientific methodological base for systems analysis, and this group is Systems and Decision Sciences. It includes our Methodology and Computer Science projects. The first leader of the methodology project was George Dantzig; the second, Tjalling Koopmans, was first succeeded briefly by Bill Jewell of Berkeley, and now for a long term, three years at least, by Michel Balinski. I am sure you will hear quite a bit about the activity of the methodology project over the next few days. I am not going into a major discussion of it, but will simply say that it has been engaged in optimization, mathematical programming in particular, and decision analysis, and in a number of other related areas.

Our computer science project has been primarily concerned with developing a computer network. As IIASA members will know, we have been experimenting with computer connections between IIASA and Moscow, IIASA and Budapest, IIASA and Bratislava, and IIASA and existing Western European networks. We have a local network linking us into computers in Vienna and in Frankfurt, which can provide access to large scale computer capacity. Our

own facilities consist of a PDP 11/45 system, which is quite adequate for many local purposes but is not the sort of thing which can handle the very large problems we occasionally face.

One of the most important projects, and in fact the first at IIASA, the one which has progressed farthest and is the largest of all, is the energy project led by W. Häfele. Again, I am sure you will hear more about it during the rest of the meeting. But I want to emphasize its major concern, that of exploring alternative energy options for the medium- and long-term future. By this we refer not to the next ten or fifteen years, but to what we will do after that: whether nuclear options, solar options, standard use of coal, geothermal, or the better use of hydrocarbon energy will be the way in which society can meet its global energy needs. The project has been concerned not only with the technologies of energy production but with the way in which these technologies imbed themselves--Professor Hafele's term--in the economy, in the environment, and in the social system. we have been taking a rather long-range view of the impact of alternative energy technologies and various transition strategies from the current energy system to a more stable long-term system.

Finally I'll mention briefly the project I have been engaged in for the last year, a state-of-the-art survey of systems analysis. We have been trying to stimulate the production of a series of monographs, to be published by John Wiley, on various aspects of systems analysis. For example, we will have a volume on multi-attribute decision making, one on computer-aided design, one on global modelling. Ultimately, we will also produce a handbook of applied systems analysis.

These remarks may provide a background for an observation that has in a sense led to this workshop. We've realized that those here—who have been dealing with energy, with environment and climate, with ecology, with food and agriculture—all face methodologically or mathematically similar problems: they are dealing with the behavior of complex systems, particularly their stability and equilibrium. And it is this striving to see how these relationships develop and what they mean that led us to invite you hear for the next few weeks.

I've said something now about the initial conditions and the current state: the future is harder to predict. IIASA got off to a good start. I think we can all agree that the future is promising. Whether our behavior is governed by differential or diffidence equations I can't say; but I can say that I hope IIASA will make a difference, and that this workshop will too.

Opening Remarks on the Proposed Activities

Koopmans: We at IIASA are delighted and gratified with the response and participation in answer to our workshop proposal. In these brief remarks I will want just to trace the origins of the proposal, both in the work of IIASA and in the much longer history of work in various fields elsewhere. I will speak of the various applications and methods fields with trepidation: I have never had the responsibility for preparing or organizing any effort that ramifies so widely in different subject matter fields as well as method fields. It will be apparent in practically everything I say that I have a very incomplete understanding of the aspects involved. With regard to ecology, my exposure has been mostly through my colleagues at IIASA. There has been an intensive collaboration between the Ecology and Methodology projects at IIASA from well before I was here, particularly in the study of the forest pest that has already been mentioned. In that study the emphasis was mostly on optimization over time in a dynamic system. George Dantzig, David Bell, John Casti, and Carlos Winkler have been very active on the method side of this work. The system studied was of course a dynamic system and therefore, along with this optimizing work, we did develop an interest in the dynamic structure of the system for its own sake. This in turn led to looking at much simpler ecological models. The people working along these lines here at IIASA that I am aware of were John Casti, William Clark, Dixon Jones, and in the summer of 1974 Terje Hansen.

This work has been continuing since I returned to the US and several papers have been circulated by members or former members of the Ecology Project, including one by Rinaldi and Gatto.

On the climate sensitivity problem, the sensitivity of climate to human intervention, my first exposure to this problem was in learning of the work that was done at the initiative of Professor Häfele, Leader of the Energy Project of IIASA, in collaboration with the British Meteorological Office in London, to test the sensitivity of climate variables in various locations to large sustained waste heat releases in various hypothetical locations. This work was based on the detailed equations of motion of the atmosphere taken from the laws of physics as applied to the atmosphere and the oceans. Computational precision was achieved by a fine resolution of space and time. subsequent conversations also with Academician Marchuk of Novosibirsk, Director of the Computer Laboratory there, first in Baden and then in Leningrad, about the methods developed by him and used in his Institute in Novosibirsk. These methods are directed towards shortcuts in the computing procedures that take advantage of the bilinear character of the equation system. After that I had the privilege of having further discussions with other meteorologists on the extent to which equilibrium concepts are helpful in climate sensitivity problems. discussions occurred first here at IIASA, at a conference at the end of April 1975, where Professor Hasselmann of a new institute in Hamburg was very informative in his remarks to me. He drew attention to models that have been made by a

number of meteorologists in which the variables are themselves defined as averages over time or space. In such models one can expect stable equilibria to arise from the computations. On the contrary, in the more complex "general circulation models" in which variables are defined with reference to a fine grid of points in space and time, any equilibrium one finds is likely to be unstable, because the very equilibrium conditions preclude the important phenomena of turbulence, including large-scale turbulence such as cyclones, cold fronts - I am not sure of the correct terminology. Much of the transport of energy and of momentum takes place through such large scale turbulence and would be missed in a computed equilibrium. After that I had the privilege to speak successively with Professor Lorenz and with Professor Charney at MIT, who is with us. Professor Charney indicated that his research led him to expect additional uses for computation of equilibria, or in any case of closed orbits in the state space, even with reference to the finer grid of the general circulation models if I understood him right. If I did not he will undoubtedly correct me, but in any case I trust he will educate us in his ideas.

I was delighted to hear on arrival here that we will have another field of application, that of chemistry, represented in the Workshop. We look forward to hearing from Professor Schuster about the applications of equilibria, closed orbits and other attractor sets in the study of biochemical evolution.

I am struck by a contrast in the role of equilibrium and other dynamic concepts in the three fields of application,

climate, ecology, chemistry, on the one hand, and in economics on the other. Certainly, in economic thought of the last fifty years in the countries with preponderantly market-oriented economies, the equilibrium concept received more attention than the systematic consideration of the dynamics of an approach to equilibrium. It is my impression that in climatology and in ecology the entire dynamics is in the center of attention, not the consideration of an equilibrium apart from the dynamics. Equilibria, closed orbits, stable or not, and the domains of attraction (the basins) in the state space from which the stable equilibria, orbits, or other attractor sets are approached, are all of interest. The central question I wish to address to the specialists in the various groups of application is the following: Does knowledge of equilibria, of the closed orbits and their stability properties provide a useful starting point for exploring what you want to know about the dynamic structure?

The mathematical terms I have been using without definition need careful spelling out and backing by theorems dealing with dynamic systems, theorems in differential topology and in ergodic theory. Professor Peter Walters has already indicated his work in this area. Our colleagues from the USSR, Professor Molchanov, Dr. Bazykin, and Dr. Penenko, use methods from this field, and Drs. Casti and Grümm from IIASA also represent these areas.

With regard to methods of computation, the choice of algorithms, the IIASA approach is to start with the problem and to try out any method or combination of methods that has a chance

of being useful. We are fortunate in having experts and practioners of various methods among our participants. In particular I want to mention the fixed point methods of calculating equilibria, that have come from economics. methods use pivot steps similar to those used in mathematical programming, but they do not involve optimization. Also, once started up these algorithms are locked into a fully determined sequence of pivot steps without the choice of a "change of basis" frequent in mathematical programming. Herbert Scarf, who is with us, is the originator of these methods. They were then developed further by Hansen, also with us, and by Harold Kuhn at Princeton, Curtis Eaves at Stanford, and other people, mostly in the U.S. and mostly coming from applied mathematics rather than from economics. There are also other methods that we want to compare or combine with the fixed point methods. Steve Robinson is our expert here on Newton methods, which have a long history, and Juncosa on extrapolation methods. Grümm, Casti, Walters, and Taranco represent mathematical systems theory, systems of differential equations of the types that arise in these various applications.

I propose that we use the time today and tomorrow morning for making brief statements to each other from the points of view of the various specialties, to open up the dialogue.

Dynamic and Equilibrium Problems in Climatology

Charney: I am not the best qualified person to talk about the problems of equilibria, stability and limit cycles in meteorology. My colleague at M.I.T., Prof. Lorenz, who was invited but was unfortunately unable to come, has done pioneering work in this field and would have been the more appropriate person. I hope to present some of his ideas during the workshop, but for this introductory talk I will present a point of view toward calculating climate which is not unrelated to his and which does involve the calculation of fixed points and limit cycles in a phase space.

Let me state the climatological problem as I see it. The earth is a spinning globe with an atmosphere and oceans whose circulations are driven by solar energy. The rotation of the earth with respect to the sun produces diurnal and semi-diurnal thermal tides in the atmosphere, but, since the radiative time constants are long, these tides are negligible, and if the surface properties of the earth were symmetric about its axis of rotation, solar heating would produce an axisymmetric circulation. Because of the earth's rotation and the tendency for conservation of angular momentum this circulation would appear as primarily zonal (east-west) with weak meridional (north-south) components. But such a circulation would never be observed, except perhaps in the tropics, because it would be unstable for wave-like perturbations propagating zonally eastward whose wave-lengths and periods would not be unlike those of the great waves and vortices

observed in the middle and upper troposphere. In the actual atmosphere the low-level motions are strongly influenced by the thermal and topographic inhomogeneities of the earth's surface and appear as the quasi-permanent high and low pressure areas of the surface weather map. The upper flow is more nearly zonal, but I have shown that this flow is unstable for one or more characteristic modes (Charney, 1947), and more recently Lorenz (1972) and Gill (1974) have shown that such modes, when they grow to finite amplitude, become unstable themselves, so that the final state of the atmosphere resembles more a fully turbulent flow than a uniformly progressing wave superimposed on a symmetric zonal flow. When one considers also the smallscale, mechanically and thermally driven, turbulence of the surface boundary-layer, it is found that the flow is turbulent over some nine or ten decades of scale, ranging from millimeters to thousands of kilometers. Fortunately for high-speed computation, the rotational constraints concentrate the energies in the larger sides, and the kinetic energy per unit horizontal wave-number, K, falls off like K⁻³ rather than, for example, like ${\rm K}^{-5/3}$ as predicted by Kolomogoroff for turbulence in the so-called inertial subrange. Because of this rapid decrease of energy with decreasing scale, the bulk of the atmosphere's energy is at wave-lengths greater than 1000km and at periods greater than one day.

But even when the energy remains primarily at large scales, the system remains intrinsically unstable; the motion is not described by stable periodic orbits in a representative phase

space; and if the initial point in the space is perturbed slightly, as by observational error, the resultant path will deviate unstably from the unperturbed path until eventually the perturbed and unperturbed states of the system will differ by as much as two states taken at random. Thus, in principle, the error in a deterministic prediction must grow until after a time there is no predictability left. Numerical experiments indicate that this time is of the order of two weeks to a month for the largest atmospheric scales and is smaller for smaller scales.

What can be said of climate as a statistical ensemble of such motions? Or of climatic change? Lorenz (1968) has discussed the various possibilities which might exist if the atmosphere-ocean system were driven by a constantly radiating sun and the conditions at the surface of the solid earth were constant. It is not obvious that there would be any climate at all; that is, the statistical moments of the atmospheric time-series from time t, to time t, might not approach a limit as $t_2 - t_1$ approaches infinity. Or if there is a climate for $t_2 \rightarrow \infty$, it might depend on the configuration of the system at the initial time t₁, i.e., the system might be intransitive, with the path spaces associated with different initial points in the phase space being disconnected. It is possible to construct highly simplified laboratory or numerical systems with strong symmetries which exhibit such intransitivity, but I shall assume that sufficiently strong random forcing always exists in the asymmetric flow to prevent such intransitivity and ask how one may calculate the climate.

One way is to calculate long time series of solutions of the equations of motion numerically for the atmosphere-ocean system (perhaps also taking into account the dynamics of polar ice) or to play Monte Carlo games with ensembles of shorter period solutions. But this, while perhaps ultimately the only way, is extremely expensive in computer time and not particularly conducive to the discovery of causal relations. Let us therefore consider climatic models which permit the direct calculation of climate without explicitly calculating time series or ensembles of transient flow.

The simplest of these is the spherically symmetric, "astrophysical" model in which horizontal asymmetries are ignored and only radiative-convective effects are taken into account. models are useful for estimating the vertical temperature structure and how it might vary with changes in gaseous or particulate constituents such as CO2, O3 and volcanic dust. Another type of one-dimensional model is obtained by considering vertically and longitudinally averaged quantities varying only with latitude. The basic dependent variable is temperature, and all quantities such as horizontal heat transport, cloud, ice-cover and albedo are determined from it. Such models often exhibit two equilibrium states, corresponding to glacial and interglacial climates, and sometimes a catastrophic third state in which all the earth is covered with ice. They are useful in focusing attention on all three components of the atmospherehydrosphere-cryosphere system, and lead to interesting speculations, such as Budyko's, on the possibility of the existence

of a stable ice-free or ice-covered Arctic basin, but they fail to take into account so many essential physical processes that their value is only to suggest what must be considered in more complete models.

The next in order of simplicity is the two-dimensional model in which quantitites are averaged longitudinally but allowed to vary latitudinally and vertically. Let us assume that the properties of the earth's surface are axisymmetric. Then a sufficiently low solar heating will produce an axisymmetric vortex, but with larger heating the vortex will become unstable and break down into asymmetric waves propagating zonally. These waves will appear as stationary flows in a coordinate system moving with the phase speed or as periodic motions in which both phase and amplitude fluctuate, i.e., as stable limit cycles in a phase space. Further increases in the solar heating will cause the translating or periodic flows to become unstable themselves and appear as truly aperiodic motions, i.e., as turbulence. All the evidence indicates that it is the latter class of flows we have to deal with. For a heating parameter, μ , which is only moderately greater than its value, μ_{c} , for instability, one may estimate the effect of the perturbation in powers of μ - μ_{c} . To first order this is equivalent to solving for the characteristic perturbation modes of the unstable flow, allowing them to interact with the mean flow but not with themselves, and determining amplitudes and interaction coefficients from a second-order energy closure condition. This was first done for simple heating and geometry by Charney (1959) and more

completely by Lorenz (1963) using truncated functional expansions. Further extensions were made by Pedlosky (1972) and Stone (1973).

The logical extension of these ideas to the highly asymmetric atmosphere-ocean system involves the calculation of the unstable, three-dimensional, stationary flow. Here one has not the criterion of axisymmetry to distinguish the stationary from the non-stationary flow. Nor, since the stationary flow, if it exists, is unstable, is it possible to calculate it, as in the symmetric case, as the asymptotic time limit of a dissipative, non-stationary flow. In an unpublished work, Milton Halem and I have calculated a stationary Hadley circulation by Newton's method, but this method appears to be too complicated and timeconsuming to apply to three dimensional flows. Not long ago I suggested to Eugenia Rivas, a former student and now an M.I.T. colleague, that perhaps a false time-variable process having the effect of rapidly damping transient flows could be found that would converge to an unstable stationary flow. She has found such a method, and it appears to have quite general applicability. She has been kind enough to supply the workshop a draft description of this method, together with some examples of its application. In particular she has applied it to an unstable two-dimensional channel flow and has shown that it does in fact yield the stationary solution.

On the assumption that some method such as Scarf's of Rivas' will permit the calculation of the unstable stationary flow as a function of a parameter μ , the next step will be to calculate the periodic (limit cycle) perturbations made for small μ - μ_{α} .

For sufficiently large μ - $\mu_{\rm C}$ one might suppose that the limit cycles themselves become unstable and approach something resembling fully-developed turbulence. At this stage, I make the, perhaps naive, conjecture that the average values and statistical moments derived from the unstable limit cycles will constitute a good approximation to those of the actual turbulent flow.* In meteorological terms, I suggest that a calculation which represents the index-cycle fluctuation between small and large amplitude wave-vortex regimes as exactly periodic, rather than merely recurrent, would capture much of the climate. This remains to be seen, but any method which avoids having to calculate the weather day-by-day for years, if not for centuries (in view of the long time constants of the oceans), would seem to merit serious consideration.

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^{*}This appears to be the case for the simple model discussed by Lorenz (1963).

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- [7] Pedlosky, Joseph "Limit cycles and unstable baroclinic waves," J. Atm. Scis., 29, 1972, 53-63.
- [8] Stone, Peter H. "The effect of large-scale eddies on climatic change," <u>J. Atm. Scis.</u>, <u>30</u>, 1973, 521-529.

Computational Aspects of the Modeling of Atmospheric Dynamics and Estimates of the Influence of Different Factors

V.V. Penenko

Abstract of Presentation

A method of construction of discrete models of dynamic atmospheric processes employing calculative variation technique is considered.

The main statement of the method is illustrated by an example of a dynamics atmospheric model on the foundation of primative hydrothermodynamics equations in diabatic approximation in an isobaric coordinate system on the sphere.

The computational algorithm is based on the splitting-up method which is used in two aspects:

- a) splitting with respect to the physical process;
- b) splitting with respect to the independent variables.

From the point of computations this method allows us to construct economical and stable algorithms.

The elements of perturbation theory are discussed for problems of the investigated class. Formulas are obtained for functional variation computations in connection with input parameter variations of the model. The construction algorithm of the perturbation theory formulas uses the solution of the adjoint problem of hydrothermodynamics.

The major steps of the numerical experiment related to modelling physical processes in the atmosphere and evaluation

of different factors incorporated in mathematical models on the dynamics of the modelling processes are presented. The general principles of the design of computational algorithms and the programs for the computer in solving problems of mathematical atmospheric modelling are discussed.

Methodological Problems in the Modeling and Analysis of Ecological Systems

C. Walters: I would like to give you an overview of basic ecological modeling and analysis problems by discussing three things. First, I will try to explain the general subject matter. This is a different perspective from that of many here, and we will almost certainly fail to understand each other if you imagine us to be, say, economists with an interest in animals. Second, I will review those structural characteristics of ecological systems which have made their analysis particularly difficult. We like to think that it is a least in part these difficulties which have kept us rather behind the rest of you in a number of methods-related areas. Finally, I'll give a brief picture of the kinds of dynamic and stability behavior which we encounter in real and model ecological systems, using as examples cases presently under investigation at IIASA and available for study at this workshop.

I. An Ecological Perspective

As you look out over a forest or field or lake or whatever, you will see a system of interacting plants and animals. In its broadest sense ecology is a science attempting to understand how these interactions are structured, how spatial and temporal patterns of species distribution are influenced by these interactions, why some creatures persist while others die out, and so on. The interactions and resulting dynamics which concern us are highly complicated and subtle, but tend to exhibit a fairly strong hierarchical structuring. At the level of most immediate reference to this workshop, the hierarchy can be viewed as one of the "eaters" and the "eaten" (i.e. of predators and prey). Further, the hierarchy is given a directional component by the fact that energy enters the system only at the lowest level of the hierarchy (plants), and flows through it (dynamically) from level to level in a manner determined by the inter-animal interactions I referred to earlier (Figure 1). (1)

Some interesting and essential work has been done on dynamics and stability properties related to the <u>structure</u> of the hierarchy⁽²⁾. Most of the interesting analysis of ecological stability properties, however, has concerned itself with the structure and behavioral properties of the preypredator and competitor-competitor interactions <u>per se</u>, largely extracted from their larger hierarchical settings. Of course, this isn't to say that the larger picture is unimportant, but rather to observe that brute force attempts to tackle the hierarchy <u>en masse</u> have been largely confusing, unproductive and crippling in terms of our analytical capabilities. With this in mind, I'll turn now to a description of the general structural properties underlying the interactions of the hierarchy, couching my presentation largely in terms of the prey-predator interactions ⁽³⁾.

II. Structural Characteristics of Ecological Interactions

Without pretending to a comprehension or detailed analysis,

I'd like to note several fundamental properties of ecological

systems which have caused us problems in their modeling and

analysis.

- (A) Nonlinearity: Ecological processes are essentially nonlinear in nature. At a fundamental level this is often due to the existence of saturation phenomena—an animal's rate of feeding will increase with available food concentration only until the animal is spending all his time feeding; higher survival rates of a parental generation will increase production of young only until all breeding sites are taken; and so on. Additionally, many biological processes—not only ecological ones—function "optimally" only under a narrow range of conditions of temperature, water availability, etc., with process rates dropping off in nonlinear ways on either side of the optimum. Although local linearization sometimes constitutes a useful approximation of system behavior over a specified range of conditions, it cannot be justified in general (4).
- (B) <u>Thresholds</u>: Ecological interactions are largely threshold phenomena. They switch on and off in an essentially discontinuous manner, with dramatic effects on system behavior. Hibernation is the most obvious example. Minimum food densities necessary to stimulate feeding response are another.
- (C) Stochastic effects: Many ecological interactions are essentially stochastic. Colonization, low density breeding, prediction search success, and such pertain here. From another

persepctive, the paramters of population interactions are distributed, even if those of individual interactions are assumed to be unique values. We know from experience that it is the tails of these parameter distributions which largely determine the long term success of populations, and one is invariably led into stochastic modeling in an effort to deal with them effectively. Finally, the environment within which ecological interactions occur provides important random inputs of such factors as weather, food supply, and so on. How far we can get through deterministic modeling of these essentially stochastic processes remains to be seen.

- earlier appears under a slightly different guise in the discrete time nature of ecological processes. Biological organisms are generally not continuous systems. They come in integral units of organisms, exhibit periods of feeding, of reproduction, of quiesence, of dispersal which are discrete and not interchangeable. Some progress has been made through use of continuous system (differential equation) approximations which treat populations as pools of biomass or energy, but these approaches are approximations and their results must be interpreted with this in mind. Several of the stability analysis properties related to this discrete time nature of ecological processes will be shown in Dr. Jones' talk later on (5).
- (E) <u>Spatial heterogeneity</u>: The ecological world is full of situations in which an interaction occurring at a given place and time effects interaction at other places only as a non-trivial function of time and location. In a sense, this is very much like the spatial problem discussed by Dr. Charney

in the climatological context. In ecology, however, the problem is complicated by the existance of a variety of poorly understood dispersal (or "diffusion") mechanisms, many of which exhibit the stochastic, discontinuous, nonlinear properties referred to above. Some work in biological oceanography has applied differential equation models of diffusion and turbulance, drawn from the fluid dynamics literature, to spatial dispersal problems in simple ecosystems (6). In more complex cases governed by biological rather than physical diffusion rules, the only workable approach has been to perform numerical simulations on a model with explicit physical grid structure. I will describe one such study later on, but the obvious disadvantage is the lack of generality inherent in the brute force approach. Nonetheless, there is no conceivable ecological problem in which the spatial component is not an essential one in the determination of stability properties and dynamic behavior.

(F) Evolving parameter structure: The ultimate problem for ecological modeling and analysis is that the so called parameters of our systems are, for the most part, actually dynamic ("control") variables which the process of natural selection is inexorably pushing towards local system "optima". I won't go any further into this for the moment, except to call your attention to the fact that even where we can identify dynamic and/or stability properties of an ecological system (or model), these must be viewed as in some sense transients. The subsequent inquiry into the parametric and even structural sensitivity of the solutions is carried out not merely to see

what would happen if we got the measures wrong, but more importantly to see what we expect the system to be doing next.

III. Dynamics and Stability Behavior of some Ecological Systems

Let me now say a few words about the behavior of preypredator systems. If we examine the state space representation of such a system, the most common case for simple experiments and models is that of Figure 2a. Here, from all starting points including some predators, the predator eats all the prey and then itself starves to death. Two trivial equilibria, unstable to positive perturbations, exist for the zero predator and zero predator-prey cases, respectively. Under different values of model parameters, and in imperfectly mixed experimental systems we get the globally stable limit cycles of Figure 2b. An additional range of parameter values yields Figure 2c's globally stable equilibrium, a situation which I may add, seems to be extremely rare in natural ecological systems. Finally, it is possible in slightly more complicated models to get multiple equilibria of the sort shown in Figure 2d. (Of course, a variety of cases are possible; one of the most interesting in an ecological sense is shown). These multiple equilbria cases arise as a result of a variety of ecological phenomena such as depensatory mortality, predator learning, or even simple minimum densities below which one or both of the species fail to reproduce. This last situation is shown for the discrete generation case in Figure 3. Note that the very small \mathbf{X}_{\min} zone is 'reflected' in a much larger portion of state space, points in which have the property of describing

trajectories which enter the X_{\min} region. Note also that the discrete nature of the prey-predator interactions allows "trajectories" to jump over the central stability region. You will find such systems described in more detail in the working paper destributed by Dixon Jones (7).

As a last example, I'd like to talk about a real system we've studied in which the spatial heterogeneities referred to earlier play an important role.

The system consists of the conifer forests of eastern

North America and an insect--the spruce budworm--which periodically undergoes tremendous epidemic outbreaks and defoliates

the forest. In a small area--say a couple of acres of trees-
the time behavior of the budworm is as shown in Figure 4.

This is analogous to the prey-predator system I discussed

earlier: the budworm goes along for a time at very low densities,

suddenly increases its density over 5 orders of magnitude,

eats all the trees, and then almost disappears as a result of

starvation. It takes 35 years or so until the forest has

recovered enough to support an additional outbreak.

If we look over the whole of eastern North America, however, the system is much less "peaky", looking more like Figure 5.

Somewhere in this region, there is almost always a local outbreak in progress, with the result that the <u>average</u> density of budworm is much more constant. What is really hapenning appears neither in Figures 4 nor 5, but rather in a physical map of eastern North America in which we trace the temporal spread of outbreaks. These turn out to be a wave or "ripple" phenomena, akin to that produced by dropping a stone in a lake. The wave

of the outbreak passess outward from its point of origin (Figure 6) giving local effects such as those shown in Figure 4 and the global ones shown in Figure 5. Restart of the cycle may occur by insects dispensing from the y=40 wave front back to the area devestated in y=O, and now recovered sufficiently to support a new outbreak. The process is, therefore, one which in any small (local) interaction can be described by a stable limit cycle of high amplitude in foliage-budworm space. These small areas are connected by dispensal of insects which leads to the large scale almost constant ("equilibrium"?) behavior of Figure 5. The very concept of "stability" seems a spatial one ... But our management interest here is precisely one of controling or influencing the local "peakyness" of the system, trying to spread the inevitable budworm damage over longer periods so that the acute free mortality caused by the outbreaks is reduced. We are trying to find a way to break up the waves of Figure 6, perhaps by reducing the amplitude of the cycle in Figure 4b. We would be very interested to know, for instance, whether there exists (even in a mathematical sense) a nontrivial stable equilibrium to the system at both the local and regional spatial level. At present, the very high dimensionality of the spatial system makes grid search techniques for such stable points hopelessly inefficient. We wonder if any of the compuational methods known to you people can help us. And we're equally interested in getting some comments from the other applied people here on what seem to be useful conceptualizations of such concepts as "stability", "equilibrium", "periodicity", in such cases

as this. We just don't have a useful way of even talking about these problems at present. And with that rather fore-lorn plea, I guess I'll $stop^{(8)(9)}$.

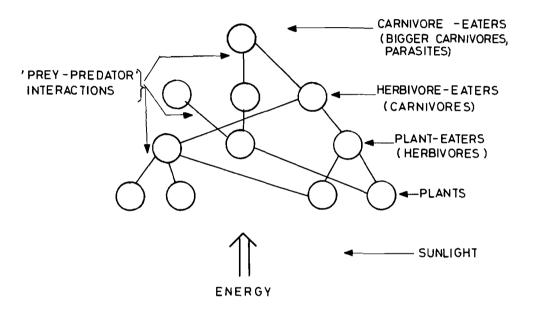
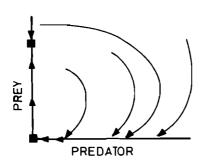


Figure 1: Hierarchical nature of ecological systems.

Note that the figure is highly oversimplified in that among other things, real systems are less strictly hierarchical, are not fixed in their interaction patterns, and include recycling (or decomposer) links from all levels back into the bottom one or two. Note also that important competitor interactions within hierarchy levels are not shown (1).



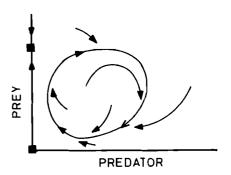
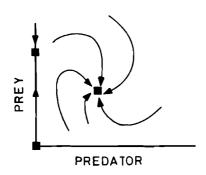


Figure 2a: Unstable.

Figure 2b: Stable limit cycle.



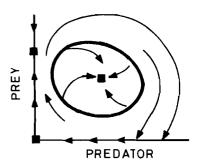


Figure 2c: Stable equilibrium.

Figure 2d: Multiple equilibria with separatrix.

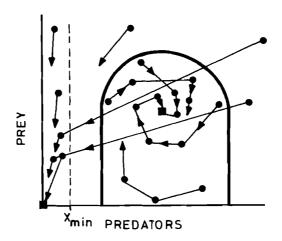


Figure 3: Multiple equilibria, caused by minimum density \mathbf{X}_{\min} below which predators fail to reproduce.

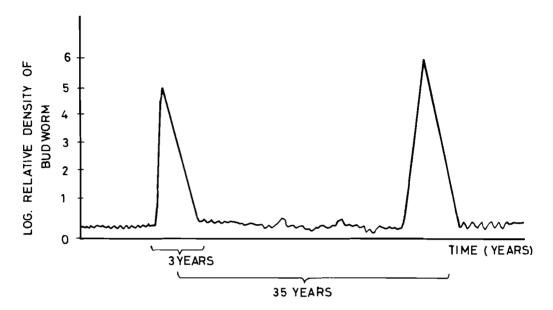


Figure 4a: Local time pattern of budworm densities.

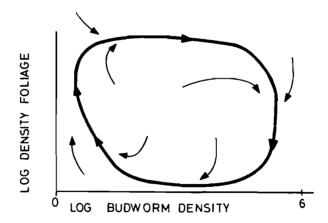


Figure 4b: State space pattern of local budworm-free interactions.

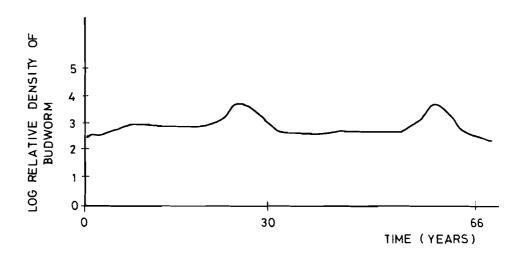


Figure 5a: Large scale time pattern of budworm densities.

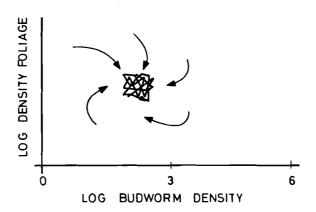


Figure 5b: State space pattern of large-scale average interactions (an apparently smaller stable limit cycle).

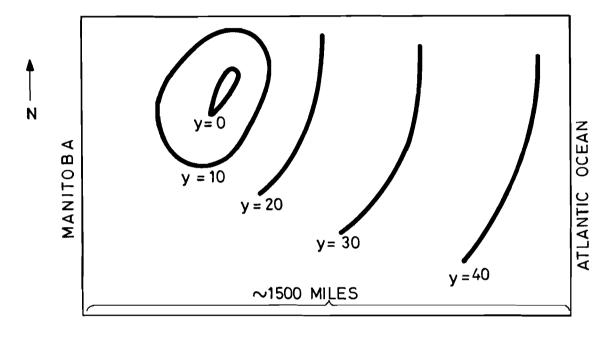


Figure 6: Physical location of budworm outbreak in Eastern North America, by year.

Notes and Selected Bibliography

- (1) See, for example, Odum, E.P., 1972, Ecology 3rd ed., Saunders, Philadelphia for a development of the hierarchy concept.
- (2) See the following for discussion of the relation between a hierarchy's structure and its stability properties.
 - May, R.M., 1973, Stability and Complexity in Model Ecosystems, Princeton University Press.
- (3) The competitor interactions are at one level structurally identical to the prey-predator ones, requiring only a change in sign of the equations. But competition studies, even at the theoretical level, have taken an approach which might be characterized as comparative statics as opposed to the comparative dynamics of most prey-predator work. See MacArthur, R.M., 1972, Geographical Ecology, Harper and Row, for the mathematical treatment of simple competition models, and May, R.M., op cit. for that of simple prey-predator ones. See also (9) below.
- (4) See Dr. Bazykin's presentations later in this volume on the relevance and implications of the Michaelis-Menton model to saturation processes.
- (5) See Maynard-Smith, J., 1974, Models in Ecology, Oxford, for a discussion of the difference in stability properties of difference and differential equation models in ecology; see also May, R.M., op cit.
- (6) See Steele, J.H., 1974, "Stability of Plankton Ecosystems," (in) M.B. Usher (ed.), <u>Ecological Stability</u>, Chapman and Hall, for a treatment of spatial effects.
- (7) See Jones, D.D., 1974, "Analysis of a Compact Prey-Predator Model." IIASA WP-74-34 for a further development of the prey-predator model.
- (8) For a further treatment of the budworm system see:
 - Morris, R.F., 1963, "The Dynamics of Epidemic Spruce Budworm Populations," Mem. Ent. Soc. Canada, 31.

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 Simulation in Systems Ecology, Simulation Council Procs. (in press). Also, IIASA RR-75-15.
- Holling, C.S., et al., 1975, "A Case Study of Forest Ecosystem Pest Management," (in) Proc. Int. Can. Conf. on Applied Systems Analysis, 1975 (in press). Also, IIASA WP-75-60.
- (9) Note added in proof: There is a large quantity of competition model literature concerned with determining how many different species can coexist (i.e. exhibit positive densities) in an ecological system at equilibrium. Much of the argument is essentially tautological, concluding only that at most there can be as many species as there are "different" resources. But in its "limiting similarity" form, the issue remains an interesting one (see MacArthur, op cit.). It would seem that this "how-many-coexisting-species-problem" is the one best suited to solution by existing fixed-point techniques.

Fixed Point Methods

H.E. Scarf

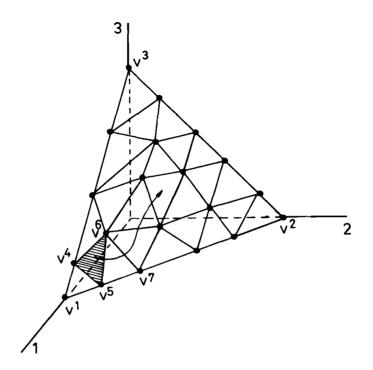
Fixed point methods have been devised to solve the general systems of equations and inequalities arising in the study of economic equilibria. The methods are completely global, making no assumptions concerning a linear approximation to the system in the neighborhood of an equilibrium nor requiring a good initial estimate of the solution as Newton's method does. One of the purposes of the present workshop has been to explore the possibility that these methods may be applied in a variety of other fields such as ecology, the study of chemical equilibria and climatology.

In order to apply fixed point methods it is customary to transform the underlying problem into one requiring the numerical determination of a fixed point of some continuous mapping of a closed, bounded convex set into itself. Let us consider an example in which the simplex

$$\{x=(x_1,x_2,x_3) \mid x_1 \ge 0, \sum_{i=1}^{3} x_i = 1\}$$
 is

mapped into itself by the continuous map $(x_1, x_2, x_3) \rightarrow (f_1(x), f_2(x), f_3(x))$ with $f_i(x) \ge 0$, and $\int\limits_{i=1}^3 f_i(x) = 1$. We

begin by constructing a simplicial subdivision of the simplex, with vertices $\{v^j\}$.



Each vertex v^j of the simplicial subdivision is given an integer label $\ell(v^j)$ contained in the set (1,2,3), and according to the following rules.

- 1. If v^j has a zero coordinate it is given the label corresponding to that coordinate (if several coordinates are zero some specific rule is required, such as selecting the first zero coordinate for the label).
- 2. If all the coordinates of v^j are positive the label is selected as one of the coordinates i, for which $f_{\nu}(v^j) \geq v_i^j.$

It is clear that a simplex in the subdivision all of whose labels are distinct, forms an approximation to a fixed point of the mapping, with the degree of the approximation dependant upon the fineness of the subdivision. An algorithm

for the determination of such a simplex (which is far less efficient than several recently developed variations) may briefly be described as follows. Begin the algorithm at the shaded simplex whose vertices are $\mathbf{v}^4, \mathbf{v}^5$ and \mathbf{v}^6 . According to our rules $\ell(\mathbf{v}^4) = 2$, and $\ell(\mathbf{v}^5) = 3$. If $\ell(\mathbf{v}^6) = 1$ the problem is over. Otherwise we move to the adjacent simplex obtained by removing that vertex whose label agrees with $\ell(\mathbf{v}^6)$, say \mathbf{v}^4 . In the triangle $(\mathbf{v}^5, \mathbf{v}^6, \mathbf{v}^7)$ we again check to see if all labels are distinct. If not, we move to the adjacent simplex determined by removing that vertex whose label agrees with $\ell(\mathbf{v}^7)$.

It may be shown that such a process never cycles, never attempts to leave the large simplex, and must therefore terminate in a finite number of iterations with a desired answer. Extensive computational experience seems to indicate that the number of iterations—and therefore the number of function evaluations—is proportional to the fineness of the grid, and to the square of the dimension of the problem. The method is therefore quite suitable for problems ranging up to say n = 20.

A number of modifications have been made in the basic method which permit us to start with an arbitrary guess of the solution rather than at a vertex of the large simplex. More importantly it is quite easy to revise the method so that the grid size is continuously decreasing rather than being prescribed in advance. These improvements have permitted us to solve problems in as many as 80 variables in relatively short periods of time with an accuracy of 10 decimal places. Moreover,

there is both mathematical and computational evidence to suggest that the final stages of the algorithm--with a very fine grid--are virtually identical with Newton's method, even though the entire algorithm is global in character.

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Description of Fixed Point Algorithms

Terje Hansen

Let us consider the following continuous mapping of the unit simplex into itself

$$y_i = f_i(x_1, ..., x_n)$$
 , $i = 1, ..., n$,

$$x_i \geq 0$$
 , $y_i \geq 0$,

for all i ,
$$\sum_{i} x_{i} = 1$$
 , $\sum_{i} y_{i} = 1$.

A fixed point of the mapping is a solution to the system of equations

$$x_i = f_i(_1, ..., x_n)$$
 , $i = 1, ..., n$.

The fixed point algorithms yield n vectors $x^1, ..., x^n$ such that

$$x_{i}^{i} \leq f_{i}(x_{i}^{i},...,x_{n}^{i})$$
, $i = 1,...,n$

and

$$|\mathbf{x}_{j}^{i} - \mathbf{x}_{j}^{k}| < \frac{1}{D}$$

for all i, j and k, where D is a large positive integer. The number of iterations required for the algorithms to terminate typically increases with n and D.

The original fixed point algorithm due to Scarf and Hansen requires the degree of accuracy to be specified in advance. For this algorithm the expected number of iterations for a specific class of problems tended to increase approximately according to the following formula:

Number of iterations required =
$$c_1 \cdot D \cdot n^2$$

where \mathbf{c}_1 is a constant. The table below which results from applying the algorithm to problems from the same general class depicts this relationship.

	Number of iterati	ons required for
	the algorithm	n to terminate
n	D = 100	D = 200
3	145	285
6	568	1120
9	1243	2490
12	2141	4260
15	3300	6605

Later versions of the fixed point algorithms due to Eaves and Merril permit a continuous refinement of accuracy. These algorithms are much more efficient than the original one proposed by Scarf and Hansen. The same kind of experiment as the

one cited above has not been done with Eaves' and Merrill's algorithms. On the basis of a variety of examples and general insight as to the behavior of these algorithms it seems reasonable to conjecture the following approximate relationship between the expected number of iterations and D and N:

Number of iterations required =
$$c_2 \cdot log D \cdot n_2$$
.

The following table depicts the relationship between the number of iterations and n in 5 applications of Eaves algorithm.

Number of iterations required for the algorithm to terminate. D = 1024

n	Number of iterations
3	35
6	144
9	340
12	546

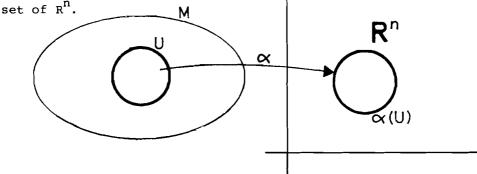
Let us conclude by saying that the amount of computation required at each iteration is essentially equivalent to evaluating the functions $f_i(x_1,\ldots,x_n)$, $(i=1,\ldots n)$.

An Outline of Structural Stability Theory

Peter Walters

This is a description of some results on structural stability of differential equations that may be useful to people at this workshop.

Let M be a C^∞ manifold of dimension n. This means M is a separable connected topological space which is covered by a family of open sets with the following properties: for each such open set U there is a homeomorphism α mapping U onto an open sub-

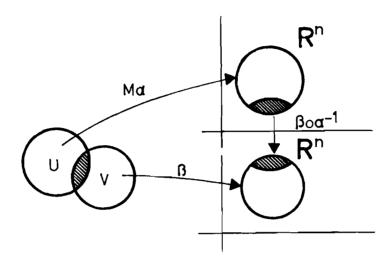


(Such a pair (U,α) is called a chart) and if (U,α) and (V,β) are charts so that $UnV \neq \emptyset$ then the map

$$\alpha (UnV) \rightarrow \beta (UnV)$$

$$y \rightarrow \beta 0\alpha^{-1}(y)$$

has partial derivatives of all orders. So a manifold is a space on which we can do differential calculus in a consistent way. Simple examples are \mathbb{R}^n , spheres, tori, and open subsets of \mathbb{R}^n .



A C^r vector field (or differential equation) on M is an assignment of a tangent vector v(x) at each point x of M in such a way that they vary smoothly in a C^r sense.

Rigorously: Let T_X^M be the collection of all tangent vectors at x. This is a vector space. Let TM be the collection of all tangent vectors to M. TM can be made into a C^∞ manifold using charts obtained naturally from those on M. If (U,α) is a chart on M let $(TU,T\alpha)$ be the corresponding chart on TM. Define $\pi:TM\to M$ by assigning to a tangent vector the point x of M where it is tangent. Then a C^T vector field is a C^T map $V:M\to TM$ so that $\pi\circ V(x)=x$ for all $x\in M$. The expression for a vector field in charts is x'=f(x). So a vector field is a first order autonomous differential equation on M.

Let $\mathscr{V}^r(M)$ denote the collection of all C r vector fields on M. $\mathscr{V}^r(M)$ is a vector space.

If M is a decent manifold, for example compact, then each $v \in \mathcal{Y}$ (M) generates a flow, i.e. there exists a C^r map ϕ_t : $RxM \to M$ such that for each x the curve $t \to \phi(t,x)$ is the solution curve of v which passes through x at time 0. Let ϕ_t : $M \to M$ denote the map $\phi_t(x) = \phi(t,x)$. Then $\phi_t(x)$ is the point the system comes to after flowing for time t from the point x. We have ϕ_0 = identity and $\phi_{t+s} = \phi_t \circ \phi_s$. We usually denote the flow by $\{\phi_t\}$. (In fact if M is a complete Riemannian manifold and v is bounded then a flow exists for v.)

So we can consider the orbit diagram or phase portrait of v. This is the diagram of solution curves on M.

We want to say a vector field v is structurally stable if nearby vector fields have similar phase portraits. We must explain "nearby" and "similar phase portraits" but first we mention some motivation for the concept of structural stability. Suppose we do some experiments and decide from them that a system satisfies a certain differential equation. This may not be the correct differential equation because of experimental error but if the correct differential equation is structurally stable and if experimental error is small, then the two equations will have "similar" phase portraits and hence the same qualitative behavior.

Let me try to explain what is meant by "similar phase portraits". If two vector fields v, w have similar phase portraits then we would like them to have the same number of equilibrium points, the same number of periodic orbits and have the same general qualitative behavior. This definition captures these features:

Two vector fields, v, w one topologically conjugate if there is a homeomorphism h of M mapping directed solution comes of v on to directed solution curves of w.

Note, that if x_0 is an equilibrium point of v, then $h(x_0)$ is an equilibrium point of w, and the image of a closed orbit of v is a closed orbit of w.

We now explain "nearby vector fields" by putting a topology on $\mathscr{V}'(M)$. We say v and w are close if they are pointwise close and so are their first derivatives. (We do this rigorously when M is compact. Choose a finite cover of M by charts (U_i, α_i) k. We can then choose an open cover V_1, \ldots, V_k of M so that $\overline{V}_i \cap U_i$ for each i. Let $(TU_i, T\alpha_i)$ k be the corresponding charts for TM. $T\alpha_i$ maps TU_i to an open subset of R^{2n} . Then

$$T\alpha_{i}^{ovo}\alpha_{i}^{-1}:\alpha_{i}^{o}(U_{i})\rightarrow R^{2n}$$

is a C^r map from an open subset of Rⁿ. Let

$$D(T\alpha_i ovo\alpha_i^{-1})(y) \epsilon L(R^n, R^{2n})$$

denote its derivative at

Put

$$\begin{aligned} ||\mathbf{v}||_{1} &= \left\{ \max_{1 \leq i \leq k} \left[\max_{\mathbf{y} \in \alpha_{i}(\overline{V}_{i})} \sup_{|\mathbf{v} \in \alpha_{i}(\overline{V}_{i})|} || \operatorname{T}\alpha_{i} \circ \operatorname{vo}\alpha_{i}^{-1}(\mathbf{y})|| \right] \right\} , \\ &= \sup_{\mathbf{y} \in \alpha_{i}(\overline{V}_{i})} || \operatorname{D}\alpha_{i} \circ \operatorname{vo}\alpha_{i}^{-1}(\mathbf{y})|| \right] \right\} . \end{aligned}$$

The sups exist as they are taken over compact sets (which is the reason for introducing the V_i 's). This is a norm which makes \mathscr{V}' (M) a separable Banach space. Then we say v and w are close if $||v-w||_1$ is small.

So the definition of structural stability is:

A vector field $v \in \mathcal{Y}'$ (M) is structurally stable if there is a neighborhood N(v) of v in \mathcal{Y}' (M) every member of which is topologically conjugate to v.

Let

S.S. (M) = all the structurally stable vector fields on M .

Then S.S.(M) is a non-empty open subset of \mathscr{V}^{\bullet} (M). The main problem is: Find necessary and sufficient conditions for a vector field to be structurally stable.

Examples.

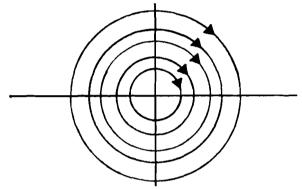
1. Simple harmonic oscillator.

$$\ddot{\mathbf{x}} = -\mathbf{x}$$

As a first order system this is

$$\dot{x} = y$$
 $\dot{y} = -x$.

The solutions are circles centered at the origin.



This is not structurally stable because any vector field topologically conjugate to v has all its orbits periodic, and we can always tilt the arrows slightly towards the origin and obtain a nearby vector field with a non-periodic orbit.

2. Van der Pol equation.

$$\ddot{x} + \varepsilon (x^2 - 1)x + x = 0 .$$

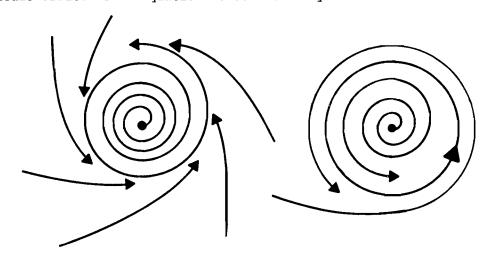
i.e.

$$\dot{x} = y$$

$$\dot{y} = -\epsilon (x^2 - 1)y - x .$$

This is one periodic orbit and every orbit outside it moves in

towards it and every orbit inside spirals out towards the periodic orbit. This equation is structurally stable.



- 3. When M is compact and of dimension two, Andronov and Pontryagin (for the 2-sphere) and Peixoto (general case) have classified S.S.(M), consider the following four conditions:
 - i) v has finitely many equilibrium points, each hyperbolic. (Hyperbolic means that the derivative of the map $\phi_{\sf t}$ has no eigenvalues of unit modulus);
 - ii) v has finitely many periodic orbits, each hyperbolic. (A periodic orbit is hyperbolic if the Poincaré first-return map has a hyperbolic fixed point);
 - iii) stable and unstable manifolds of equilibrium points and
 periodic orbits meet transversally when they intersect.
 (This means no tangency is allowed between stable and
 unstable manifolds);
 - iv) the non-wandering points are just the equilibrium points
 together with the points on the periodic orbits. (A

point x is non-wandering if for each open neighborhood U of x and each T > 0 there is a t > T with $\phi_t U \cap U \neq \phi$). If v has all these properties it is called a Morse-Smale system. Let M.S.(M) denote those vector fields having all these properties. Then if

$$dim(M) = 2$$
 , $MS(M) = SS(M)$,

- i.e. the Morse-Smale systems are exactly the structurally stable ones. If dim $M \geq 2$ then M.S.(M) \subset S.S.(M), (Palis-Smale). The structural stability of Morse-Smale systems comes from the hyperbolic nature of the equilibrium points and periodic orbits. We now define some vector fields where hyperbolic behavior occurs at each point.
- 4. Let M be compact and let || || denote a Riemannien metric on M (this gives a norm to each tangent space).

is an Anosov vector field if

- a) $v(x) \neq 0$ all $x \in M$ (i.e. no equilibrium points);
- b) at each point \mathbf{x} of M the vector space $\mathbf{T}_{\mathbf{x}}^{\mathsf{M}}$ is a direct sum of three linear subspaces

$$T_{\mathbf{x}}M = E_{\mathbf{x}}^{O} \oplus E_{\mathbf{x}}^{S} \oplus E_{\mathbf{x}}^{U}$$

such that $E_{\mathbf{x}}^{O}$ is the one-dimensional space spanned by $v(\mathbf{x})$ and

$$T\phi_t(E_x^s) = E_{\phi_t(x)}^s$$
, $T\phi_t(E_x^u) = E_{\phi_t(x)}^u$.

c) E_x^s is contracting exponentially and E_x^u is expanding exponentially, i.e. \mathfrak{z} a > 0 and c > 0 such that

$$||T\phi_{+}\xi|| \leq Ce^{-at}||\xi||$$

if t > 0 and $\xi \in E_{\mathbf{X}}^{\mathbf{S}}$ and

$$||T\phi_{-t}\eta|| \le Ce^{-at} ||\eta||$$

if t > 0 and $\eta \in E_X^S$. Let A(M) denote the collection of all Anosov systems on M. Then Anosov proved:

- (i) A(M) is an open subset of $C^{r}(M)$
- (ii) A(M)⊂SS(M)
- (iii) If X is a compact manifold of negative curvature the geodesic glow on TX = M is an Anosov vector field.
- 5. Smale observed that the stability probably arises from the hyperbolic behavior at non-wandering points. Let $\Omega(v)$ denote the non-wandering points of v. v is said to satisfy axiom A if
- i) $\Omega(\mathbf{v}) = \Omega_1 \cup \Omega_2$ where Ω_1 consists of a finite number of equilibrium points all hyperbolic, and Ω_2 contains no equilibrium points.
- ii) The periodic orbits are dense in Ω_2 and for each point ${\bf x}$ of Ω_2 we have

$$T_{x}M = E_{x}^{O} \oplus E_{x}^{S} \oplus E_{x}^{U}$$

satisfying b) and c) as in 4.

If v satisfies Axiom A then the stable mainfolds $W^S(x) = \{y \in M | \text{distance } (\phi_t y, \phi_t x) \to 0 \text{ as } t \to +\infty \}$ are submanifolds of M for $x \in \Omega$ and $W^S(x)$ is tangent to E_X^S at x. Similarly, $W_{(x)}^U = \{z \in M | \text{distance } (\phi_t y, \phi_t x) \to 0 \text{ as } t \to -\infty \}$ is tangent to E_X^U if $x \in \Omega$. v is said to satisfy the strong transverality condition if whenever $W^U(x)$ and $W^S(y)$ intersect then they do so transversally. There is the theorem: If v satisfies Axiom A and the strong transversality condition then v is structurally stable (Robbin, Robinson). It is conjectured that the converse is true.

A reference which is probably the best beginning reading is:

L. Markus, "Lectures on Differentiable Dynamics," Regional Conference Series in Math., A.M.S. Monograph No.3.

OPENING PLENARY SESSION, SCHLOSS, JULY 22, AM

Extrapolation Methods for Equilibria Calculations

M. L. Juncosa

When asked to give this expository talk, I had a problem of decision relating to what was implied by here in this workshop the concept of equilibrium as it appears in different contexts, economic, dynamical system, chemical climate, ecological, statistical, etc., and what exprapolation methods for their calculation meant.

Mathematically, an equilibrium point of a transformation, G, mapping some general space (usually a Banach space) into itself, has been defined as equivalent to a fixed point (x = G(x)) of the mapping. Its relation to a "steady state" of a system is close when one generalizes the notion of a point to include a cycle or a periodic sequence of iterates of the transformation G of the point x.

At any rate, many problems of equilibrium calculations can be subsumed by the problem of solving the equation F(x)=0 or the equation x=G(x) where F is a mapping from a Banach space to another while G is from one into itself. For computational considerations, these spaces are usually n-dimensional Euclidean spaces.

At various times it may be more advantageous to deal with F(x) = 0 rather than x = G(x) and vice versa; but they are equivalent to each other. (E.g., if F(x) = 0 and if A is any appropriate non-singular linear transformation, then x = x + AF(x) = G(x).)

Extrapolation methods are <u>local</u> rather than <u>global</u> methods, i.e., from local information on local values of the function, evaluated at an estimate of a solution in a single point method and at several successive estimates in multi-point methods, an extrapolation (which could be an interpolation in some multi-point method) to a hopefully better estimate of a solution is made. However, without some general topological conditions on the transformation extrapolation methods can at best, only produce local solutions. Notwithstanding that at times they may be inferior to global methods in robustness and in domain of convergence, when they converge, they usually do with a much greater rate than those that are global, e.g., search methods.

Of the single step, or single point, extrapolation methods for solving equations the simplest in concept, though not necessarily computationally the fastest, is Newton's (Raphson's) method which consists in linear extrapolation from a functional value at an estimate to a zero of the extrapolation for the hopefully improved estimate.

Thus, for the problem of seeking a solution of a system of non-linear equations F(x)=0, starting with an initial estimate x_0 , the algorithm is to improve the n-th estimate successfully by solving the linear system

$$F(x_n) + F'(x_n)(x_{n+1} - x_n) = 0$$

where $F'(x_n)$ is the Jacobian matrix of F with respect to x (whenever it exists) evaluated at the point x.

When it converges to a simple root, the process does so rapidly, i.e. it has second order convergence:

$$||x_{n+1} - x|| \le K||x_n - x||^2$$

where K is some positive constant. At each step its computational price is the evaluation of F and F' at x_n and the inversion of F'.

Quadratic extrapolation methods, e.g., the method of tangent hyperbolas, in one dimension going back at least to Halley of comet fame, has third order convergence when converging to a simple root. However, except in one dimension, generalizations to higher dimensions (e.g., that of Mertvekova to a Banach space) involve not only computations of F and F' and inversion of F' but usually also the coumputation of F'' and the inversion of an additional operator. The computation of F'' is usually a factor of the dimension more costly than that of F'. For the cheaper price of two successive Newton extrapolations considered as one step one gets fourth order convergence.

Thus, in higher dimensions, from the computational point of view, one generally should not consider methods of any higher order than second for solving equations.

Computational considerations usually outweigh considerations of rate of convergence alone and have led to variants of Newton's method such as keeping the initial $F'(x_0)$ throughout the sequence of iterations or least for some fixed number of them before recomputing F'. Other alternatives involve linear extrapolations in other directions other than those determined by $F'(x_n)$.

This makes them usually multi-step methods which may be considered as generalized secant methods. Their rates of convergence are, for simple roots, better than first order but not quite second order:

$$||x_{n+1} - x|| < \kappa ||x_n - x|| ||x_{n-1} - x||$$
.

Wolfe, Comm. ACM., 1959, and Barnes, Brit. Comp. Journal, 1965, and others have produced generalized secant method algorithms.

I'll go no further on this topic, Newton's Method and variants being the topic of the next speaker.

Regarding a problem in the form x = G(x), to which, as noted above, F(x) = 0 is equivalent, the typical extrapolation is successive substitutions or Picard's method for differential and integral equations or relaxation methods for linear equations, as functional iterations are variously called.

Computational operations per extrapolation are about as cheap as one could expect, but are, when convergent, slow, i.e., one has first order convergence:

$$||x_{n+1} - x|| \le K||x_n - x||$$

where 0 < K < 1. To improve the convergence rate a process known as the Aitken-Steffensen-Householder-Ostiowski- δ^2 -extrapolation process can be used. (Ostrowski, Solution of Equations and Systems of Equations, Acad. Press, 1960). In one dimension at the cost of no new functional evaluations, only some trifling

arithmetic, higher convergence rates can be obtained through the use of the formula

$$x_{n+1} = \frac{x_n x_{n-2} - x_{n-1}^2}{x_n - 2x_{n-1} + x_{n-2}}$$

where x_{n-1} and x_n are successive iterates of G on x_{n-2} . One of the derivations of this formula is to apply the secant procedure to x - G(x) = 0.

Not only does this process usually (but not always; counter examples are possible) have a higher rate of convergence than linear but often converts a divergent iteration of G into a convergent one and also often has a larger domain of convergence.

Investigating the convergence of the δ^2 -extrapolation procedure Ostrowski (1960) has considered it as a problem of investigating the rate of convergence of iterations of

$$\Psi(x) = \frac{xG(G(x)) - G^2(x)}{G(G(x)) - 2G(x) + x}$$

to a fixed point $\xi = \Psi(\xi)$. If

I:
$$E(x) = \frac{G(x) - \xi - \alpha(x - \xi)}{|x - \xi|^{\lambda}}$$
, $\lambda > 1$, $\alpha(\alpha - 1) \neq 0$,

he showed that

a) E bounded as
$$x \to \xi \Rightarrow \Psi(x) - \xi = \mathcal{O}(|x - \xi|^{\lambda})$$

b) E + 0 as x +
$$\xi \Rightarrow \Psi(x) - \xi = o(|x - \xi|)^{2\lambda - 1}$$

(If $\alpha > 0$, if the approach of x to ξ is one-sided, then so are the conclusions of a) and b).)

II: If
$$\alpha = 0$$
, $\lambda > 1$ and $E(x) = (G(x) - \xi)/|x - \xi|^{\lambda}$,

then

a) E bounded as
$$x + \xi \Rightarrow \Psi(x) - \xi = \mathcal{O}(|x - \xi|^{2\lambda - 1})$$

b)
$$E \rightarrow 0$$
 as $x \rightarrow \xi \Rightarrow \Psi(x) - \xi = o(|x - \xi|^{2\lambda - 1})$.

III: If $\alpha = 1$, G'(x) continuous near ξ and $G'(x) - 1 = T(x) |x|^{\lambda-1}$, where $T(x) \to \lambda \neq 0$, either as $x \uparrow \xi$ or $x \downarrow \xi$, then $\Psi'(\xi) = 1 - \frac{1}{\lambda}$ and ξ is a point of attraction of $\Psi(x)$ from the corresponding side.

To generalize the δ^2 -extrapolation process to higher dimensions, one may attempt δ^2 -extrapolation in each discussion. With empirical success, Noble has applied it to a solution of nonlinear integral equation discretized to a system of non-linear transcendental equations and Bellman, Kagiwada, and Kalaba to the zero boundary-value problem for $u'' = e^u$ on (0,1) discretized for computation.

However it is easy to construct a very simple example in two dimensions, viz.,

$$\begin{pmatrix} x \\ y \end{pmatrix} = \frac{1}{2} \begin{pmatrix} y \\ -x \end{pmatrix} ,$$

whose fixed point, the origin, has no circle of convergence in which component-wise δ^2 -extrapolation converges for all points in the circle.

This suggests that a generalization to higher dimensions probably requires simultaneous involvement of all component equations. Thus, in the spirit of some one-dimensional derivations of the δ^2 -extrapolation procedure and multi-dimensional derivations of generalized secant methods, one multi-dimensional δ^2 -extrapolation process is given by

$$(I - Kn)(x_{n+1}^* - x_n) = x_{n+1} - x_n$$

where \mathbf{x}_{n+1}^* is the more rapidly converging improvement to \mathbf{x}_{n+1} , I is the unit matrix in the Euclidean space of, say, k dimensions of the problem and \mathbf{K}_n is determined by solving the linear matrix equation

$$K_n[x_n - x_{n-1}, x_{n-1} - x_{n-2}, \dots, x_{n-k+1} - x_{n-k}^*]$$

=
$$[x_{n+1} - x_n, x_n - x_{n-1}, \dots, x_{n-k+2} - x_{n-k+1}]$$
,

where bracketed expressions are k x k matrices whose columns are successive differences of the indicated vectors determined from a sequence of k + 1 iterates of G on \mathbf{x}_{n-k}^* the previously improved iterate.

Thus in k dimensions this generalized δ^2 -extrapolation process has as its iteration function

$$\Psi(x) = G^{k}(x) - [G^{k}(x) - G^{k-1}(x), \dots, G(x) - x]$$

$$\cdot [G^{k+1}(x) - 2G^{k}(x) + G^{k-1}(x), \dots, G^{2}(x) - 2G(x) + x]^{-1}$$

$$\cdot [G^{k+1}(x) - G(x)] ,$$

where $G^{i}(x)$ is the i-th iteration of G on x.

Some of the results of Ostrowski can be obtained for this generalization under similar conditions.

Convergence Theorem: Let G(x) be differentiable and its Jacobian satisfy a Lipschitz condition in a neighborhood of $\xi (= G(\xi))$ and, furthermore, that its value, J, at $x = \xi$ satisfies the condition that $J \cdot (J - I)$ is non-singular. Then $\Psi(x)$ is a contraction mapping in a neighborhood of ξ .

Theorem: With the same hypothesis of the convergence theorem, then for λ > 1

$$G(x) = \xi + J \cdot (x - \xi) + \mathcal{O}(||x - \xi||^{\lambda})$$

implies

$$\Psi(\mathbf{x}) = \xi + \mathcal{O}(||\mathbf{x} - \xi||^{\lambda})$$

and

$$G(x) = \xi + J(x - \xi) + o(||x - \xi||^{\lambda})$$

implies

$$\Psi(\mathbf{x}) = \xi + o(||\mathbf{x} - \xi||^{\lambda}) .$$

Theorem: If the Jacobian of G is Lipschitzian near ξ and vanishes at ξ then for λ > 1

$$G(x) = \xi + \mathcal{O}(||x - \xi||^{\lambda})$$

implies

$$\Psi(\mathbf{x}) = \xi + \mathcal{O}(||\mathbf{x} - \xi||^{\lambda^{k} + \lambda - 1})$$

and

$$G(x) = \xi + o(||x - \xi||^{\lambda})$$

implies

$$\Psi(x) = \xi + o(||x - \xi||^{\lambda^{k} + \lambda - 1})$$
.

Other generalizations in Banach spaces have been given by J.W. Schmidt, ZAMM 1966, S. Yu. Ulm, USSR Jour. Comp. Math. and Math. Physics 1964, and Ion Pavaloiu, Rev. Rom. de Math. Purer et Appl., B. T. Polyak, USSR Jour. Comp. Math. and Math. Physics 1964.

There can be some computational problems associated with this method. Let us go back to the equations for the k-dimensional $\delta^{\,2}$ iteration function, $\Psi(\mathbf{x})\,.\,$ Look at the equation defining K_n , particularly at the matrix multiplying $\boldsymbol{K}_{\boldsymbol{n}}$ and also the right hand side matrix. As \boldsymbol{n} gets larger, the consecutive values of \boldsymbol{x}_{n} get closer and closer together, so the columns in these matrices get closer and closer to Therefore, there has to be an appropriate upscaling of the columns of these matrices in order to get a practical, computational solution for $\mathbf{K}_{\mathbf{n}}$. This is something like saying that K_{n} times a nearly null matrix is equal to another nearly null matrix, if there is no upscaling, a highly unstable computational situation. But of course, that appears in the one dimensional form as well. Here we have the same kind of situation. Here we have the numerator and denominator close to zero. From the computational point of view, one must pay attention to these problems of sensitivities, to achieve meaningful results.

Newton's Method for Systems of Nonlinear Equations

Stephen M. Robinson

I. Introduction

Newton's method is a device for the numerical solution of certain nonlinear operator equations; it may also be adapted for use with inequalities. Although it can be used for equations in either finite-dimensional or infinite-dimensional spaces, our consideration here will be restricted to finite-dimensional systems of the form

$$f(x) = 0 ,$$

where f is a differentiable function from \mathbb{R}^n into itself. The Newton method is based on the very simple observation that, near a point \mathbf{x}_0 ϵ \mathbb{R}^n , the linearized function

$$Lf(x_0, x) := f(x_0) + f'(x_0)(x - x_0)$$

is a good approximation to f, and on the fact that linear systems are usually easier to solve than nonlinear ones. The algorithm, in its simplest form, proceeds as follows:

- 1. Start with some $x_0 \in \mathbb{R}^n$; set k := 0.
- 2. Given x_k , find some x_{k+1} (if any exists) such that $Lf(x_k, x_{k+1}) = 0.$
- 3. Decide whether to stop; if not, set k := k + 1 and go to Step 2.

General-purpose programs for implementing this algorithm exist, and are often worth using for problems not possessing special structure nor presenting unusual difficulties (see Section IV for some discussion of common difficulties). One such program is described in [4]; it includes provisions for automatic determination of error bounds for the computed solution.

II. Convergence properties

The fundamental convergence result for Newton's method in this form states that if f' is Lipschitzian in a neighborhood of a simple zero \mathbf{x}_* of f (i.e., a point satisfying $\mathbf{f}(\mathbf{x}_*) = 0$ and for which $\mathbf{f}'(\mathbf{x}_*)$ is invertible), then there is some neighborhood \mathbf{Q} of \mathbf{x}_* such that for each initial point \mathbf{x}_0 \mathbf{c} \mathbf{Q} , the sequence $\{\mathbf{x}_k\}$ exists and converges R-quadratically to \mathbf{x}_* : that is, there are some constants \mathbf{q} and \mathbf{q} , with \mathbf{q} \mathbf{c} (0,1), such that for all \mathbf{k} ,

$$||\mathbf{x}_{k} - \mathbf{x}_{*}|| \leq \alpha \gamma^{(2^{k})}$$
,

where $||\cdot||$ is an arbitrary, but fixed, norm on \mathbb{R}^n . Thus, the sequence of errors $\{||\mathbf{x}_0 - \mathbf{x}_*||, ||\mathbf{x}_1 - \mathbf{x}_*||, \ldots\}$ is majorized by the sequence $\{\alpha\gamma, \alpha\gamma^2, \alpha\gamma^4, \alpha\gamma^8, \alpha\gamma^{16}, \ldots\}$, which converges rapidly to zero. This extremely fast convergence is one of the principal reasons for using the Newton method.

Actually, an even stronger convergence result holds for this method: the result, due to L.V. Kantorovich, permits one to infer the existence of \mathbf{x}_* from data at the initial point \mathbf{x}_0

and from a knowledge of the Lipschitz constant for f'. For a statement of this theorem, see Theorem 12.6.2 of [5], and for somewhat improved error bounds see [1]. The book [5] is a very complete reference for many kinds of procedures for the solution of systems of nonlinear equations; also, an excellent expository treatment of Newton's method (and of other solution techniques) can be found in [7]. The theorem of Kantorovich appears in his famous monograph of 1948 [3].

III. Variants and extensions

Many variants of Newton's method have been devised, some designed to reduce the computational labor involved in the use of the method, others to "tailor" the algorithm to a specific type of problem (such as finding an unconstrained local minimizer of a real-valued function). Many of these algorithms are treated in [5]; see also the comments at the end of Section IV below.

In addition, the method can be extended to solve mixed systems of inequalities and equations; substantially the same type of convergence analysis is possible as in the case of equations alone. For details, see [6], [8].

IV. Possible difficulties in using Newton's method

There are two major sources of possible difficulty in applying the Newton method to a practical problem: one relates to the choice of a starting value, and the other to the computations which must be done in Step 2 (basically, setting up

and solving an n x n system of linear equations). As noted above in the discussion of convergence, the initial point \mathbf{x}_0 must be "close enough" to the solution in order for the convergence theorems to apply. As a practical matter, it has been found that starting points which are too far away from \mathbf{x}_* to satisfy the theoretical requirements very often still yield convergent sequences; however, randomly selected starting points cannot be expected to result in convergence. It should be kept in mind also that for a problem having several solutions, the choice of a starting point will determine to which (if any) of these solutions the sequence of iterates will converge.

The other major difficulty involves the work in Step 2 of the algorithm: for each k, one must compute $f'(x_k)$ (an n x n matrix) as well as $f(x_k)$, then solve an n x n system of linear equations. The difficulty of computing $f'(x_k)$ obviously is compounded if the partial derivatives involved are difficult to compute, of if n is large; on the other hand, in the latter case $f'(x_y)$ may be sparse, so that only a few elements have to be computed. Complicated partial derivatives can be dealt with by using an automatic (analytic) differentiation program (see, e.g., [2]). Another way of dealing with this difficulty is to avoid computing $f'(x_{\nu})$, and to use instead an approximation, often obtained numerically from values of the function f. The so-called secant methods are based on this idea; for details about these methods, see [5]. Sometimes one can approximate the inverse of $f'(x_k)$, so that no equations need be solved; however, if this is not done or if one computes $f'(x_k)$ directly,

then it will be necessary to solve a system of n linear equations in n unknowns. If n is not too large (say, not more than a few hundred) and if the equations are not ill-conditioned (i.e., if their solutions are not excessively sensitive to small variations in the data) this should not be too difficult with a good code for solving linear equations. On the other hand, the presence of ill-conditioning of the requirement to solve very large systems usually means that special precautions need to be taken to ensure that the computed solution is not very different from the true answer. Ill-conditioning can be visualized, in the case of a single equation, by thinking of a function whose graph is nearly horizontal close to a zero. functions do not determine their zeros very well, and this is often an indication that the mathematical formulation of the original physical or economic problem could better have been done in a different way; alternatively, the trouble may be inherent in the problem, but in either case a re-examination of the problem and its formulation is generally in order. The solution of large linear systems, on the other hand, is a problem of numerical analysis, and the techniques used are likely to be highly problem-dependent: one generally tries to take as much advantage as possible of the special form (if any) of $f'(x_{\nu})$, and different solution techniques (e.g., iterative methods [9]) may be employed for large systems than would be used for small ones.

Another devise for avoiding the repetive solution of linear systems is to use a fixed matrix in place of $f'(x_k)$, or

alternatively to recompute $f'(x_k)$ only periodically, instead of at each step. In either case one has to carry out the factorization of the resulting matrix only the first time it is used; at succeeding steps the previously-computed factors are employed, together with the current value of $f(x_k)$, to compute x_{k+1} in only $O(n^2)$ operations instead of $O(n^3)$ as would be the case if a new matrix had been used. Unless one uses the (generally unknown) matrix $f'(x_*)$, the iteration with a fixed matrix will not be quadratically convergent; however, if the matrix is close to $f'(x_*)$ then the method is likely to converge at a rather fast, even though linear, rate. Thus, for problems whose derivatives do not change quickly around x_* , this technique may well be worth trying. For a rigorous discussion and convergence results, see [5, §§10.2, 12.6.1].

Material Added in Response to Discussants Remarks

Let me briefly indicate some extensions of the Newton method. So far we have been talking about problems of the following form: f(x) = 0. This is, of course, one way in which one can express an equilibrium condition for many problems.

On the other hand, there are problems in which inequalities are essential to the description of the equilibrium. One of them might be the kind of non-linear problem which was discussed by Professor Scarf -- $g(x) \le 0$, $x \le 0$, $x \le 0$. Now this kind of problem, although it can be represented in the form of a system of non-linear equations, is probably not naturally

so represented. One would ask then if there are Newton methods for this kind of problem. There are, in fact, Newton methods for solving systems of inequalities and equations, such as the following: g(x) = 0 and $h(x) \le 0$, and these proceed in a manner not too different from the classical Newton method. is not all that different and the convergence analysis is pretty much the same.* The difficulty is that when doing the Newton method we require a regularity condition, namely that the derivative of f at $\overline{\mathbf{x}}$ be non-singular. Now there is a corresponding regularity condition for this kind of system, which is necessary or seems to be necessary in order to obtain a convergence theory for methods for solving this type of equation-inequality system. Unfortunately, problems like the nonlinear complementarity problem never satisfy such a regularity condition. other words, such systems are always singular in the sense of not being able to satisfy the condition that one seems to require for convergence of this type of method. This suggests to me that we need to know considerably more about the dynamics of solutions of systems of inequalities of this particular form under changes in the functions, because notice that in the Newton method what we are really doing is introducing a certain perturbation into the function, which changes it a little bit. Near x_0 the linearized function is very much like f(x) and it's from the knowledge of the dynamics of the solution set of the linearized system versus the original system, that we get the convergence theory of Newton's method. I know of no such information about complementarity problems or

^{*}For example, see the Kantorovich-type theorem in [8].

equilibrium problems in general. We do have some information about systems of inequalities if they satisfy a regularity condition, but we do not have such information about equilibrium systems, and I would suggest that this might be a very, very important topic of study, among other reasons for the development of more effective computational methods.

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OPENING PLENARY SESSION, GARRET, JULY 22, PM

Self-Organizing Chemical Systems

Peter Schuster

The usual problem to find fixed points in chemical systems corresponding to chemical equilibrium or stationary states is rather simple with respect to its mathematical background since in the meaningful range of variables in general only one stable fixed point does occur. Recently, people became interested in more complex chemical systems showing ranges of instability, multiple fixed points and limit cycle oscillations. This kind of system turned out to be able, furthermore, to fulfill a number of necessary requirements to start a process of self-organization which is of crucial importance for any theory on the origin of life. In this lecture I will restrict myself to this kind of system.

I. Origin of the problem

In the early stages of biochemical evolution exclusively biopolymers or their precursors with random or nearly random sequences were present. There was <u>no</u> structural or functional correlation between them. The step of the development we are interested in here leads from these random polymers to the first ordered entity which we can recognize as a precursor of the most primitive organisms showing the three most important characteristics of living systems: 1) Metabolism or energy flux; 2) Multiplication of self-instructed reproduction; and 3) Mutations or small errors in the reproduction. Eigen [1,2] formulated for this purpose a theory of Darwinian evolution

on a molecular level and we will follow the mathematical background briefly here. Selection on the molecular level will be formulated as an optimization process in discrete steps, which correspond to favorable mutations. The function to be optimized, the value function ω , is related to the dynamics of the self-organizing system or more basically to the physiochemical properties of the macromolecules themselves.

II. Mathematical background of the problem

There are two sets of macromolecules $\{S_i\}$ and $\{P_i\}$ characterized by different sequences and properties. S_i corresponds to a macromolecule acting as information storage for the synthesis of a macromolecule P_i , which is the active biochemical catalyst, roughly speaking S_i are the precursors of nucleic acids and P_i the precursors of proteins. We start with two sets of populations $\{X_i\}$ and $\{Y_i\}$, which are functions of t and represent the number of polymers at a given time.

In the first period of the self-organizing process at maximum a few copies of a given sequence will be present:

$$X_{i}(t) = 0,1,2,...$$
, $Y_{i}(t) = 0,1,2,...$

A stochastic treatment of the dynamics for such a system capable of self-instructed replication (1) and degradation (2)

$$S_{i} + \sum_{v} \lambda_{v} A_{v} \xrightarrow{f_{i}} 2A \tag{1}$$

$$S_{i} \xrightarrow{d_{i}} \sum_{v} \lambda_{v} B_{v}$$
 (2)

$$B_{y} + \text{energy} \rightarrow \rightarrow A_{y}$$
 (3)

coupled to an "energy bath" (3) shows, that after some time only a few sequences will be present, but now each sequence in a large number of copies: $X_i >> 10^3$. Bartholomay [3] has treated a similar problem in biology by Doob's matrix technique for Markov chains. For further details see the given reference.

Now we can assume $X_{\underline{i}}$ to be a quasi-continuous variable and formulate a set of differential equations, which describe the evolution of the system (4):

$$\dot{X}_{i} = (F_{i} - D_{i})X_{i} + \sum_{k=i}^{\Sigma} \varepsilon_{ik}X_{k}$$
 (4)

 ϵ_{ik} are small terms in general, representing the probability for a spontaneous mutation from \mathbf{X}_k to \mathbf{X}_i . \mathbf{F}_i and \mathbf{D}_i in almost all realistic cases are complicated functions of many kinds of small molecules and macromolecules present. They represent the growth and degradation terms of \mathbf{S}_i .

The growth term F_i can be split in a production rate A_i and a quality factor Q_i representing the accuracy of reproduction (Q_i = 1 means no errors, probability for mutation = 0). Now we can formulate new quantities the excess production E_i , the mean excess production \overline{E} and the value function ω_i (5-8):

$$\mathbf{F}_{\mathbf{i}} = \mathbf{A}_{\mathbf{i}} \cdot \mathbf{Q}_{\mathbf{i}} \tag{5}$$

$$E_{i} = A_{i} - D_{i} \tag{6}$$

$$\widehat{\mathbf{E}} = \sum_{\mathbf{i}} \mathbf{X}_{\mathbf{i}} \mathbf{E}_{\mathbf{i}} / \sum_{\mathbf{i}} \mathbf{X}_{\mathbf{i}}$$
 (7)

$$\omega_{i} = A_{i}Q_{i} - D_{i} . \qquad (8)$$

Inserting these expressions in (4) we obtain a new set of differential equations (9), which is very suitable for a discussion of selection on a molecular level:

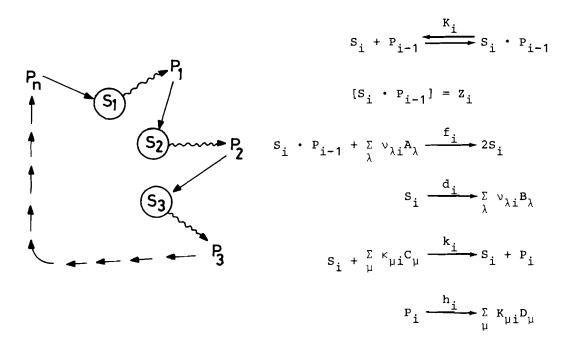
$$\dot{X}_{i} = (\omega_{i} - \overline{E})X_{i} . \tag{9}$$

Since $\overline{E}(t)$ does not depend on a particular species a population is increasing if $\omega_i > \overline{E}$ and decreasing if $\omega_i < \overline{E}$. The function to be optimized in the procedure of evolution is ω_i . Concrete examples are presented in [1] and [2]. For a given set of macromolecules $\{S_i\}$ the sequence with maximum value of ω_i will be selected. ω_i , however, might well depend on the concentrations of other macromolecules present in the system. In this case the result of the selection is not unique and will depend on initial conditions. Model systems were chosen in order to learn more about growth properties, selection mechanisms and probabilities for survival of mutations.

III. Model Systems

Out of all model systems discussed until now [1,4] we choose here one representative example. A set of n sequences

 $\{S_i, i = 1,...,n\}$ is dynamically correlated to a set of n sequences of type $\{P_i, i = 1,...,n\}$. According to the following set of reaction equations forming a catalytic cycle:



These equations can be easily translated into the following system of coupled ordinary differential equations (10-12):

$$\dot{X}_{i} = f_{i}Z_{i} - d_{i}(X_{i} - Z_{i})$$
 (10)

$$\dot{Y}_{i} = k_{i}(X_{i} - Z_{i}) - h_{i}(Y_{i} - Z_{i+1})$$
 (11)

$$z_{i} = \frac{x_{i} + y_{i-1} + x_{i}}{2} (1 - \sqrt{1 - \frac{4x_{i}y_{i-1}}{(x_{i} + y_{i-1} + x_{i})^{2}}}) . (12)$$

The general type of solution was found to depend on the concentrations of macromolecules present and on the number of members in the cycle.

a) low concentration limit: x_i , $y_{i-1} \ll K_i$ simplified equations $\dot{x}_i = f_i x_i x_{i-1} - \frac{x_i}{c_0} \sum_{j=1}^n f_j x_j x_{j-1}$ $f_i = f_2 = \dots = f_n = 1 .$

Normal modes around central fixed points: $X_i > 0$

$$W_{1} = -\gamma$$

$$W_{j} = \lambda_{n}^{-j+1} \cdot \gamma ; \quad j = 2,...,n$$

$$\lambda_{n} = \exp(-2\pi i/n)$$

n = 2, stable fixed point, no oscillation

n = 3, fixed point, damped oscillations

- ${\tt n}$ = 4, metastable fixed point, undamped oscillations with small amplitudes
- n \geq 5, unstable fixed point, limit cycles or more complicated attractors
 - b) high concentration limit: X_i , $Y_{i-1} >> K_i$ simplified equations $X_i = f_i X_{i-1} \frac{X_i}{c_o} \sum_{j=1}^n f_j \cdot X_{j-1}$ $f_i = f_2 = \dots = f_n = 1 .$

Normal modes around central fixed point: $X_i > 0$

$$W_{j} = -1 + \lambda_{n}^{-j} , \quad j = 1, 2, \dots, n$$

$$\lambda_{n} = \exp(-2\pi i/n) .$$

Stable fixed points, n > 3 damped oscillations.

IV. Conclusions

Different growth terms were found to have substantial influence on the selective behavior of the system. Linear growth terms, $\omega_i \neq \omega_i (X_i, X_i, Y_i)$, lead to selection of the species with best or "fittest" physicochemical properties. The number of sequences present at the initial conditions (X_i^0) has no influence on the outcome provided X_i^0 is above the level of stochastic threshold. Favorable mutants are tolerated at the beginning and finally selected. Systems with nonlinear growth terms, however, show a different behavior. After one species has been selected a favorable mutant has no chance to survive. Thereby decisions "once and for all" along the path of evolution are made and indeed there are some hints that those decisions occurring in the early historical evolution of life on earth - unique genetic code, unique chirality in all organisms known. kind of model discussed here would allow such "once and for all" decisions at the beginning of evolution (low concentration limit) and then finally switch to a Darwinian type of evolution based on a mutation-selection mechanism.

v. References

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WORKING SESSIONS, GARRET, JULY 23-30

Bifurcations and the Appearance of Attracting Tori, July 23

H.R. Grümm

In the last years, there has been renewed interest in getting a qualitative understanding of turbulence on the basis of the behavior of the system in the neighborhood of a range attractor. This approach was mainly pioneered by D. Ruelle with the collaboration of R. Bowen and F. Takens. This presentation intends to give an outline of these ideas and to show how they can be applied to the purpose of the workshop. Rigorous proofs will be mostly omitted. From the beginning I want to stress that in my opinion it is possible to apply the following to a range of questions considered in the workshop, mainly climatological models, chemical evolution models and ecological food chains.

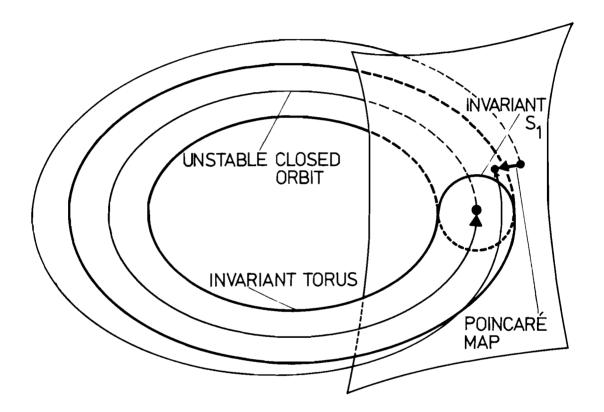
Let us assume we are given a family of continuous-time dynamical systems, given by $\dot{x}=F_{\mu}(x)$, on a possibly infinite-dimensional manifold (to include problems with partial spatial derivative). μ is a parameter describing a "driving force" of the system, like solar inradiation or energy input to a food chain. We assume further that for $\mu=0$ there is a stable fixed point x_0 of F_{μ} corresponding to a stationary state of the system which becomes unstable for larger μ . ($\mu > \mu_0 > 0$) As μ increases from 0, the implicit function theorem gives the existence of a fixed point x_{μ} of F_{μ} , close to x_0 .

We look for the spectrum of the operator $DF_{11}(x_{11})*:$ if

^{*}This is a shorthand notation for the matrix $\left(\frac{\partial F^{\dot{1}}}{\partial x_{\dot{1}}}\right)$.

 $\mu \leq 0$ certain μ_1 , it will still lie in the left half-plane, 0 "slightly perturbed" stationary state. Suppose that at $\mu = \mu_1$ a pair of complex-conjugate eigenvalues crosses the imaginary axis. An argument due to Hopf and extended by Ruelle and Takens shows that, depending on the sign of a higher order term in the expansion of F_{μ} at x_{μ} , an attracting closed orbit appears. One says that the fixed point bifurcates to form this closed orbit. At μ just above the critical level μ_1 , it is approximately located in the plane spanned by the eigenvectors of $DF_{\mu}\left(x_{\mu}\right)$ belonging to the two unstable eigenvalues.

As μ increases further, more pairs of eigenvalues will cross the imaginary axis and the closed orbit will become unstable. One can look at its Poincaré map: at a certain $\mu=\mu_2$ the center fixed point becomes unstable and again depending on the sign condition an attracting manifold diffeomorphic to a circle and invariant under the Poincaré map will branch off. This of course corresponds to the formation of a 2-torus around the original fixed point.



By these arguments it becomes very plausible, and further confirmation can be obtained by a theorem by Hirsh and Shub, that in general the following happens: if k pairs of eigenvalues have crossed the imaginary axis and the sign conditions are right, an invariant attracting k-torus will form. This can be understood as a Hopf bifurcation in each of the k planes spanned by eigenvectors belonging to a pair of eigenvalues.

The flow on the attracting torus will describe the behavior of the system in a neighborhood of the unstable fixed point. We can describe only its "generic" characteristics. If the torus is 2-dimensional, by Peixoto's theorem there will be a finite number of attracting closed orbits on it. So almost every point in the vicinity will tend to one of these closed orbits. This is, for instance, the situation found in the Lorenz model (see presentation by Professor Charney).

For tori of higher dimension, the situation is very complicated. One can make only general statements on the generic behavior. A quasi-periodic flow (k periods of oscillation on the k-torus, with irrational ratios so that every orbit would be dense) is not to be expected since such a dynamic system can be changed by arbitrarily small modifications into one without this characteristic.* Indeed, we can modify it in such a way that it shows a strange attractor. The random-like and irregular behavior associated with a strange attractor may well be the reason for the well-known nature of turbulence. Compare the situation in Lorenz' model.

^{*}There is another argument against the appearance of quasiperiodic flow in turbulence: the time-correlation functions would not go to zero for such a flow, as they are observed to do.

A last added idea: the location of the unstable elements (fixed point or closed orbit) may be interesting for time-averages, like in climatology. The average of an observable over the attractor might be roughly approximated by its value at the fixed point or its average over the closed orbit.

Note added in proof:

For clarification I want to explain some terms in this paper. An <u>attractor</u> is a closed set A in phase space, invariant under the flow such that there exists a neighborhood U of A which will contract to A in the future and no closed subset of A has this property (i.e., stable fixed point, limit cycles). A <u>strange attractor</u> is an attractor which is not a smooth manifold. The simplest example of a strange attractor looks locally like the product of a cantor discontinuum and an interval.

The best reference for this field is the original paper of Ruelle and Takens: "On the Nature of Turbulence", Comm. Math. Phys., 1971.

A Geometrical View of Fixed Point Algorithms

Herbert E. Scarf

This lecture, given by Scarf on July 24, covered the contents of Sections 1, 2, 3 and some examples taken from Section 4, of Curtis Eaves and Herbert Scarf, "The Solution of Systems of Piecewise Linear Equations," Cowles Foundation Discussion Paper No. 390, February 27, 1975, to be published in Mathematics of Operations Research, Volume 1, and is included with the permission of that journal.

I. Introduction

In this paper we study, from a geometrical point of view, the solutions of systems of piecewise linear equations involving one more variable than equations. As our examples will indicate, virtually all of the fixed point and complementary pivot algorithms, as well as a number of related techniques which have been developed over the last decade can be cast in this framework (Lemke and Howson [15], Lemke [16], Scarf [20, 21], Scarf and Hansen [22], Kuhn [13, 14], Eaves [4, 6, 8], Shapley [24], Merrill [18], Katzenelson [12], Fujisawa and Kuh [10], and Chein and Kuh [1]). This geometrical setting leads naturally to an index theory—analogous to that of differential topology—which is of considerable importance in the study of uniqueness and monotonicity of these algorithms. Examples of the use of index theory in computation have recently been given by Kuhn [14], Shapley [23] and Lemke [17].

In the development of our ideas we have been strongly influenced by the lucid exposition of differential topology presented by Milnor [18], and by a number of stimulating conversations with Stephen Smale. Other important sources are the exposition of index theory on discrete structures given by Fan [19], and the constructive proof of the piecewise linear non retraction theorem of Hirsch [11].

In the interests of simplicity we have avoided the most general presentation and restricted our attention to a small number of well known applications. For example, the domain on which our equations are defined will be the union of a finite number of compact convex polyhedra. With some cost in simplicity the domain could equally well have been a non-compact orientied piecewise linear manifold. We have also omitted from the paper applications such as the non-linear complementarity problem in which index theory is extremely useful. These will be described in subsequent publications.

II. Piecewise Linear Mappings of Polyhedra

We shall be concerned with a set of points P in Rⁿ⁺¹ which is the union of a finite number of compact convex polyhedra,

P₁, P₂,...,P_k each of which is assumed to be of dimension (n + 1), and no two of which have an interior point in common. The term polyhedron, with the adjective "convex" omitted, will be used to describe such a set. The convex polyhedra used in constructing P wil be referred to as the pieces of the polyhedron.

Figure 1 represents a somewhat extreme example of such a polyhedron. As the figure illustrates, the polyhedron P need not be convex even though it is composed of convex pieces. It need not be connected or for that matter simply connected, and moreover the intersection of two adjacent pieces of P need not

be a full face of either polyhedron as they are assumed to be in a simplicial subdivision.

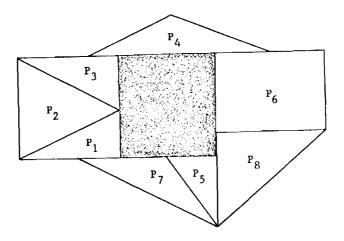


Figure 1.

An example which is more typical of those arising in the application of our techniques is given in Figure 2. In this example the polyhedron P is the product of an interval with the

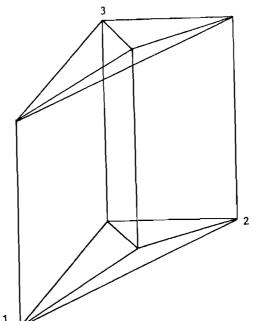


Figure 2.

simplex $S = \{(x_1, x_2) | x_i \ge 0, x_1 + x_2 \le 1\}$. The pieces $\{P_i\}$ are obtained by taking the product of this interval with each n-simplex in a simplicial subdivision of S.

We consider now a mapping F of the polyhedron P into Euclidian space R^n , which is assumed to be linear $(F(\alpha x + (1 - \alpha)x') = \alpha F(x) + (1 - \alpha)F(x'))$ in each piece P_i and continuous in P. In each of our applications the polyhedron P and the mapping F will be defined by the nature of the problem and we shall be concerned with solutions to the system of equations

$$F(x) = c$$

for a specific vector c in Rⁿ.

In order to motivate the subsequent arguments let us begin with a few intuitive and not quite rigorous remarks about the character of the set of solutions to such a system. In each piece of linearity P_i the mapping F(x) is linear with a maximal rank of n, since the mapping is into R^n . If the mapping is, in fact, of rank n in a given piece of linearity then the intersection

$$F^{-1}(c) \cap P_i$$
,

if it is not empty, is generally a straight line segment touching two distince faces of P_i of dimension n.

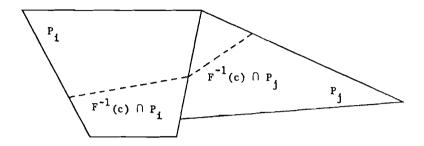


Figure 3.

Consider an adjacent piece of linearity P_j whose intersection with P_i contains a single point of $F^{-1}(c)$. Since the mapping is continuous on the common boundary P_i and P_j we expect in general that

$$F^{-1}(c) \cap P_{i}$$

will be a straight line segment in the piece of linearity P_j which fits together continuously with the corresponding segment in P_i . We shall see shortly what technical points must be examined in detail in order to make this type of argument precise. For the moment, however, these remarks seem to suggest that the set of solutions $F^{-1}(c)$ can be obtained by traversing a series of straight line segments from one piece of linearity P_i to an adjacent one.

Since the polyhedron is composed of a finite number of bounded pieces, there are essentially two types of curves (by a curve we mean a homeomorph of closed bounded interval or a circle) that can arise in this fashion. One possiblity is that the process of moving from one piece of linearity to an adjacent piece will terminate by reaching the boundary of the polyhedron P. Since movement is possible in two directions this would imply a curve touching the boundary of P in two distinct points; we shall call such a curve a path. This case is illustrated in Figure 4, in which the dashed line represents $F^{-1}(c)$.

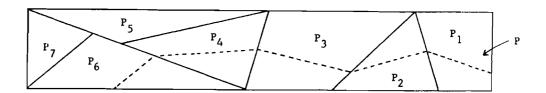


Figure 4.

Another possibility that may arise by continuing the straight line segments is the generation of a closed curve or loop which has no intersection with the boundary of P. Figure 5 illustrates a possibility in which the set of solutions $F^{-1}(c)$ contains such a loop in addition to a path terminating in a pair of boundary points of P.

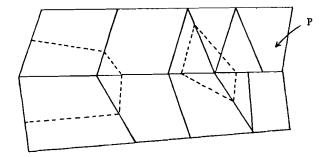


Figure 5.

These rough arguments suggest that the set of solutions to F(x) = c will either be empty or be a disjoint union of a finite number of paths and loops. As we shall see, this important conclusion will generally be correct. However, the problem may occasionally become degenerate for specific choices of the function F and vector c and produce a set of solutions more complex than that described above.

For example, we may be working in a piece of linearity P_i in which the rank of F(x) is less than n. In such a region the solutions of F(x) = c may very well form a set of dimension strictly larger than one. Another illustration of difficulty arises if for some piece of linearity P_i the set $P_i \cap F^{-1}(c)$ lies fully in the boundary of P_i .

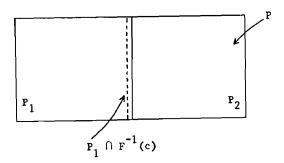


Figure 6.

A final example occurs when the set $F^{-1}(c)$ intersects the boundary of a piece of linearity P_i in some face of dimension less than n. As Figure 7 illustrates, this case may produce a bifurcation of the path in two different directions. The common

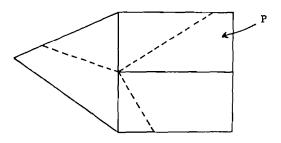


Figure 7.

feature of these examples, and in fact of all difficulties caused by degeneracy, is the fact that F(x) = c has a solution on some face of dimension less than n, of a piece of linearity.

In the next section we shall use this idea to impose a condition on the basic problem which avoids degeneracy and permits us to establish the main theorem characterizing the set of solutions to F(x) = c.

It may be appropriate at this point to provide a formal definition of the terms "path" and "loop," which have been used in the previous discussion.

2.1. [Definition] A path is a curve in P with two endpoints, each of which lies in the boundary of P and whose intersection with each piece of linearity is either empty or a straight
line segment. A loop is a closed curve with no endpoints whose
intersection with each piece of linearity is either empty or a
straight line segment.

Figures 4 and 5 illustrate paths and loops; Figure 6 a path but of the type we shall avoid, and in Figure 7 the dotted set is neither a path nor a loop.

III. The Main Theorem

We are given a polyhedron P in Rⁿ⁺¹ and a piecewise linear mapping F which carries P into Rⁿ. The following definition employs a modification, which is suitable to our purposes, of well known terminology used in differential topology.

3.1. [Definition] A vector c in R^n is a <u>degenerate</u> value of $F: P \rightarrow R^n$ if there is an x in P lying in a face of dimension

less than n of some piece of linearity P_i , for which F(x) = c. A vector c which is not a degenerate value is called a <u>regular</u> value of the mapping.

Consider the following simple illustration of this definition.

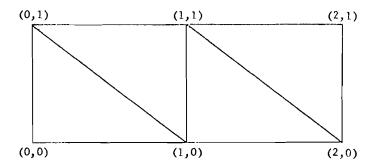


Figure 8.

The polyhedron P is composed of four triangles in \mathbb{R}^2 . The mapping into \mathbb{R}^1 is given by $F(x_1,x_2)=x_1+x_2$. According to the definition the degenerate values are those taken on at the six 0-dimensional faces (vertices), and are therefore given by (0, 1, 2, 3). The regular values of the mapping consist therefore of all points in \mathbb{R}^1 other than these four values—illustrating the fact that vectors in \mathbb{R}^n which are <u>not</u> assumed by F are considered to be regular values. We also see that degenerate values can be assumed on faces of higher dimension; for example, the value 1 is assumed by F on the entire face connecting (0, 1) and (1, 0).

We shall now provide a complete description of the set of solutions to F(x) = c, when c is a regular value of the map. We shall organize the argument by demonstrating the following preliminary lemma.

3.2. [Lemma] Let P_i be a piece of linearity, let c be a regular value of F, and assume that $P_i \cap F^{-1}(c)$ is not empty. Then $P_i \cap F^{-1}(c)$ consists of a single straight line segment whose endpoints are interior to two distinct faces of dimension n of P_i .

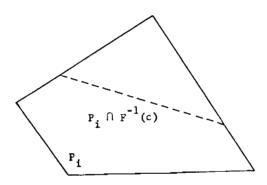


Figure 9.

In order to demonstrate this lemma let us assume that $F(x) = Ax + b \text{ in } P_i \text{ with A an } nx(n+1) \text{ matrix. First of all}$ let us remark that the matrix A has rank n. Otherwise the value c is assumed on a face of dimension n - 1 of P_i , contradicting the assumption that c is a regular value.

Since A is of rank n the solutions to $A\mathbf{x}$ + b = c in $P_{\mathbf{i}}$ form a straight line segment. The line segment cannot be fully

contained in any face of dimension n of P_i , since extending it would then enable us to reach a face of dimension n - 1. Its endpoints must therefore be contained in the interiors of two distinct faces of P_i . This demonstrates the lemma.

We are now prepared to prove the major theorem characterizing the set of solutions to F(x) = c, where c is a regular value.

3.3. [Theorem] Let $F: P \to R^n$ be continuous and linear in each piece P_i , and let c be a regular value. Then the set of solutions of F(x) = c is a finite disjoint union of paths, each of which intersects the boundary of P in precisely two points, and loops, which have no intersection with the boundary of P.

The proof of Theorem 3.3. is, of course, an immediate consequence of the arguments of the previous section combined with Lemma 3.2. If $F^{-1}(c)$ has a non-empty intersection with a piece P_i , then this intersection will consist of a straight line segment touching two faces of dimension n of P_i , and no lower dimensional face either of P_i or of any adjacent piece of linearity. If either endpoint of this line segment is not on the boundary of p it will be contained in precisely one other piece of linearity, say P_j . (The fact that this endpoint is contained in at most one other piece of linearity is the feature which assures that paths do not bifurcate as in Figure 7.) But then $P_j \cap F^{-1}(c)$ will not be empty and will consist of a similar straight line segment.

This process will either produce a path which intersects the boundary of P in two distinct points, or a path which returns

to itself and is therefore a loop. This provides us with one component of the set of solutions to F(x) = c. If there is another piece of linearity which intersects $F^{-1}(c)$ we continue by constructing an additional component. Since there are a finite number of such pieces of process of constructing paths and loops will ultimately terminate. This demonstrates Theorem 3.3.

This characterization of the set of solutions to F(x) = c is valid only if c is a regular value of the mapping; if c is degenerate the corresponding set may be considerably more complex. In applying Theorem 3.3. it will be necessary to avoid degenerate values, which, as the following theorem indicates, form a negligible subset of R^n .

3.4. [Theorem] The set of degenerate values is a closed subset of \mathbb{R}^n , contained in a finite union of (n-1) dimensional hyperplanes.

This theorem, analogous to Sard's theorem in the case of differentiable manifolds, is an immediate consequence of the definition of a degenerate value to be the image of a point x lying in an n-1 dimensional face of some piece of linearity. There are a finite number of such faces, each of which is carried by F into a closed subset of an n-1 dimensional hyperplane in \mathbb{R}^n .

Theorem 3.4., in the form stated above, is not quite suitable for most of our applications since a value c is considered to be a regular value whenever $F^{-1}(c)$ is empty. While the degenerate values form a small subset of R^n , they need not form a small

subset of the image of P under F. For example, if F maps all of P onto the same vector then all values for which $F^{-1}(c)$ is not empty, will be degenerate. The following theorem is a sharpening of Theorem 3.4., which is more appropriate for our purposes.

3.5. [Theorem] Let Q be a face of dimension n of a piece P_i , and let x be interior to this face. Assume that the image of Q under the mapping F is of dimension n. Then any relative neighborhood of x on the face Q, contains points x' for which c' = F(x') is regular.

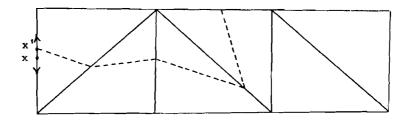


Figure 10.

The hypothesis of Theorem 3.5. imply that any neighborhood of x, on Q, will be mapped into a set of dimension n by the linear transformation obtained by restricting F to Q. Since the set of degenerate values of F is a set of dimension n-1 or less, there will be many values of x' in this neighborhood, whose image is a regular value of F.

Theorem 3.3. permits us to treat degeneracy by a slight perturbation of the vector c, as is customary in linear programming. (See any standard reference which discusses the resolution of degeneracy in linear programming.)

IV. Examples of the General Method

In the present section we shall illustrate the significance of our characterization of the set of solutions to F(x) = c by applying this result to a series of examples which have played an important role in the development of fixed point computational techniques. There are many other examples which we have chosen not to discuss in this paper.

Example 1

Our first example is that of "integer labelling," one of the earliest techniques for the numerical approximation of a fixed point of a continuous mapping of the simplex into itself. For simplicity of exposition we shall take the particular form of this method described in Chapter 7 of [16]. (Also see Cohen [2] and Eaves [4, 5].)

Consider a simplicial subdivision of the simplex S = {x = x₁, n \\ \dots, x_m) | x_i \geq 0, \Sigma x_i \leq 1} which is arbitrary, aside from the assumption that the only vertices of the subdivision lying on the boundary of S are

$$v^0 = (0,0,...,0)$$

 $v^1 = (1,0,...,0)$

$$v^{2} = (0,1,...,0)$$

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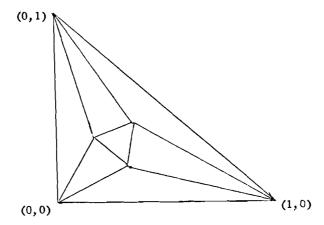


Figure 11.

Let every vertex v of this subdivision be given an integer label $\ell(v)$ selected from the set $(0,1,\ldots,n)$. The label associated with a given vertex will typically be assigned on the basis of some underlying mapping of the simplex into itself. For our purposes, however, the labelling can be considered to be arbitrary, aside from the proviso that v^i receive the label i, for $i=0,1,\ldots,n$.

We shall show that Theorem 3.3. can be employed, in the present context, to demonstrate the existence of at least one simplex in the subdivision all of whose labels are distinct.

This conclusion can be viewed, of course, as a simplified form of Sperner's lemma.

The conventional computational procedure for determining such a simplex starts out with the unique simplex in the subdivision containing the vertices v^1, \ldots, v^n and the additional vertex v^j . If the label associated with v^j is 0, the process terminates. Otherwise we remove that vertex of the simplex say v^k whose label agrees with that of v^j . A new vertex v^k is introduced, where the vertices $v^1, \ldots, v^n, v^j, v^k$, with v^k omitted, form a simplex in the subdivision. If the label associated with v^k is 0 the process terminates; otherwise we continue by removing the vertex whose label agrees with that of v^k .

At each iteration we are presented with a simplex whose vertices bear the labels 1,2,...,n. Of the two vertices with the same label, we remove the one which has not just be introduced. The argument that the algorithm does not cycle and must terminate with a simplex of the desired type may be found in the previously cited reference.

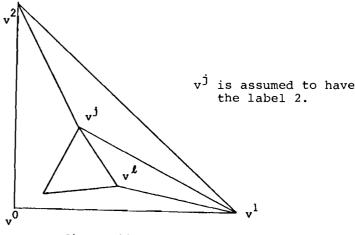


Figure 12.

In order to place the problem in our context we make the following definition.

- 4.1. [Definition] Define a continuous map $f : S \rightarrow S$ of the simplex into itself as follows:
- 1. Let v be any vertex of the simplicial subdivision, and let $\ell(v)$ = i be the integer label associated with v. We then define f(v) to be v^i .
- 2. We extend the definition of f to the entire simplex by requiring f to be linear in each simplex of the subdivision of S.

With this definition the function f is piecewise linear in S, and because of the special structure of the subdivision it is easy to see that f(x) is the identity map $(f(x) \equiv x)$ on the boundary of S. In order to demonstrate the existence of at least one completely labelled simplex it is clearly sufficient to show that for any vector c, <u>interior</u> to the simplex S there will exist a vector x, for which

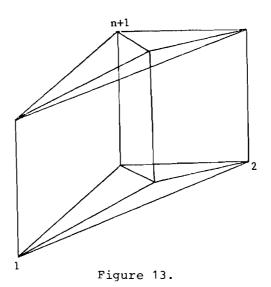
f(x) = c.

The vertices of that simplex in the subdivision which contains x will certainly bear distinct labels. For if the label i is omitted, then the image of each vertex in the simplex will be on that face of S whose ith coordinate is zero (or on the face n Σ x_i = 1, if i = 0). f(x) will therefore lie on the boundary of S, contradicting the assumption that c is an interior point.

Conversely, if the vertices of a particular simplex in the subdivision bear distinct labels then it is easy to see that the system of equations f(x) = c, has a solution contained in that simplex.

We begin by defining a polyhedron P in R^{n+1} .

4.2. [Definition] The polyhedron P is defined to be the product of the simplex S with the closed interval [0,1], i.e. $\{(x_1,\ldots,x_n,x_{n+1}) \mid x_i \geq 0, \ \sum\limits_{1} x_i \leq 1, \ \text{and} \ x_{n+1} \leq 1\}.$ The pieces $P_1,P_2,\ldots,P_k \text{ of P are obtained by taking the product of an arbitrary n-simplex in the subdivision of S with the same closed interval [0,1]. }$



The following definition will provide us with a function $F(x_1,...,x_n,x_{n+1})$ to which Theorem 3.3. can be applied.

4.3. [Definition] Let d be the vector in \mathbb{R}^n all of whose coordinates are unity. We define

$$F(x_1,...,x_n,x_{n+1}) \equiv f(x_1,...,x_n) - x_{n+1}d.$$

F is a continuous map of P into R^n which is linear in each piece of the polyhedron P. Our purpose is to show that for an arbitrary vector c, interior to the simplex S, $F^{-1}(c)$ will intersect that face of P on which $\mathbf{x}_{n+1} = 0$.

Let c be a vector interior to S and let us examine the intersection of $F^{-1}(c)$ with the other faces of P. First of all we remark that $F^{-1}(c)$ cannot intersect that face of P on which $x_{n+1} = 1$. This would imply

$$f(x_1,...,x_n) - d = c$$
,

which is impossible, since $f_i(x) \le 1$, d = (1,1,...,1) and $c_i > 0$ for all i.

On the remaining faces of P, other than the two ends of the prism, we know that $f(x) \equiv x$. A vector x in $F^{-1}(c)$ which is on such a face will therefore satisfy

$$x - x_{n+1}d = c ,$$

the unique solution of which is given by

$$(x_1^*,...,x_n^*) = c + \frac{(1 - \sum_{i=1}^{n} c_i)d}{n}$$
,
 $x_{n+1}^* = \frac{(1 - \sum_{i=1}^{n} c_i)}{n}$.

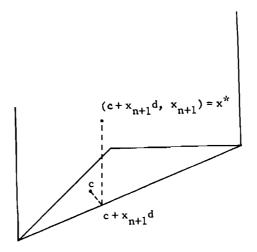


Figure 14.

We have therefore demonstrated the important conclusion that if c is interior to S, the equations F(x) = c have precisely one solution on the boundary of P other than on that face where $x_{n+1} = 0$. But if c is a regular value of the mapping F, Theorem 3.3. can be invoked to produce a path starting from x^* . Since the path must terminate at some other boundary point of P, there must be a vector on the bottom face of P for which F(x) = c. As we have already seen, this demonstrates the existence of a completely labelled simplex.

In order for this argument to be complete we need only show that there exists at least one vector c, interior to S, which is a regular value of the mapping F. But this follows immediately from Theorem 3.5. and the observation that F maps the face of P on which $\sum_{i=1}^{n} x_{i} = 1$ onto an n-dimensional subset of \mathbb{R}^{n} .

Let us examine the path generated from x* and terminating with a solution to the problem in somewhat greater detail.

Since c is a regular value this path will move from one piece of lineariy to an adjacent one by passing through the interior of their common face Q.

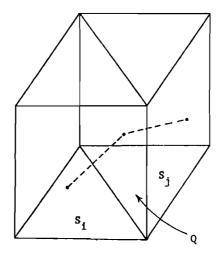


Figure 15.

The face Q is the produce of the interval [0,1] with the intersection of two adjacent simplices in the simplicial subdivision of S, say S_i and S_j . It is easy to see, however, that the n vertices common to S_i and S_j must together bear all of the labels 1,2,...,n. For if the i^{th} such label were missing it would follow that $f_i(x) = 0$ on this common intersection, which contradicts

$$f(x_1,...,x_n) - x_{n+1}d = c$$
.

We see, therefore, that the projection of our path to the lower face of P moves through simplices each of which has vertices which together bear all the labels 1,2,...,n, and which do not bear the label zero until the process terminates. Each such simplex must have a single duplicated label belonging to that vertex which is being removed in passing to the next simplex. The sequence of simplices is therefore identical with that produced by the conventional algorithm, described at the beginning of the example.

It may also be instructive to remark that a second algorithm to F(x) = c on the face $x_{n+1} = 0$ would generate a second path lying on $F^{-1}(c)$ which would, of necessity, return to this face. This permits us to arrive at the well known conclusion asserting the existence of an odd number of solutions to f(x) = c. (See Figure 16.)

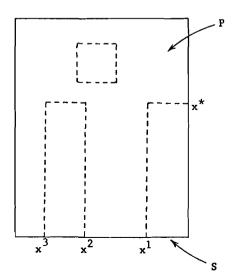


Figure 16.

Example 2

As our second example we shall indicate a way in which fixed point methods based on "vector" labels (a version of the main theorem in the monograph by Scarf and Hansen [22]) rather than integer labels may be placed in the general framework of this paper. We begin with a simplicial subdivision of the simplex

$$s = \{x = (x_1, ..., x_n) | x_i \ge 0, \frac{n}{2} x_i = 1\}$$
.

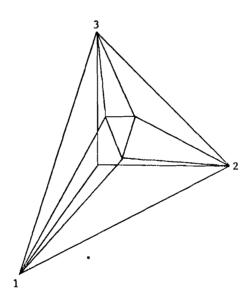


Figure 17.

Let the vertices of the subdivision be denoted by $v^1, v^2, \dots, v^n, v^{n+1}, \dots, v^k,$ where

$$v^{1} = (1,0,...,0)$$
 $v^{2} = (0,1,...,0)$
 \vdots
 \vdots
 $v^{n} = (0,0,...,0)$

For simplicity of exposition we make the assumption that no vertices of this subdivision, other than the first n vertices, lie on the boundary of S.

Each vertex v^j will have associated with it a vector $f(v^j)$ contained in \mathbb{R}^n . In practice this association is determined by the particular problem being solved; for our purposes, however, we may consider the vector labels to be completely arbitrary aside from the assumption that

$$f(v^{i}) = v^{i}$$
 , for $i = 1, 2, ..., n$.

In addition to this assignment of vector labels a specific positive vector \mathbf{c} in $\mathbf{R}^{\mathbf{n}}$ is given.

By a solution to this problem we mean the determination of a particular simplex in the subdivision, with vertices $^{j}_{v}^{$

$$\alpha_{j_1} f(v^{j_1}) + \alpha_{j_2} F(v^{j_2}) + ... + \alpha_{j_n} f(v^{j_n}) = c$$
,

have a non-negative solution $(\alpha_{j_1}, \alpha_{j_2}, \ldots, \alpha_{j_n})$. In order to guarantee that such a solution does indeed exist it is sufficient to make the following assumption.

4.4. [Assumption] Let $\alpha = (\alpha_1, \alpha_2, \dots, \alpha_k)$ be non-negative and satisfy

$$\sum_{j=1}^{k} \alpha_{j} f(v^{j}) \leq 0 .$$

Then $\alpha = 0$.

To cast this problem in our general form we begin by defining a function f(x) taking the non-negative orthant of R^n into R^n , as follows:

- 1. $f(v^{j})$ = the vector label associated with v^{j} for any vertex of the subdivisions;
 - 2. f(x) is linear in each simplex of the subdivision S, and
- 3. f(x) is homogeneous of degree 1, i.e., f(λx) = $\lambda f(x)$ for any $\lambda \geq 0$.

According to this definition, f(x) is therefore linear in each cone with vertex at the origin whose half-rays pass through a particular simplex in the subdivision of S. Because of the special assignment of vector labels to the vertices v^1, \ldots, v^n , the function is the identity $(f(x) \equiv x)$ on the boundary of the non-negative orthant of R^n . Moreover, assumption 4.4. implies that for no non-negative vector x, other than the zero vector, will f(x) be ≤ 0 .

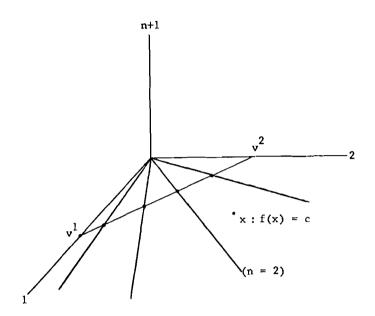


Figure 18.

It should be clear that solving the vector labelling problem is simply equivalent to the determination of a non-negative vector \mathbf{x} for which

$$f(x) = c$$
.

The particular simplex in the subdivision involved in the solution is then obtained by intersecting the ray from the origin through x with the simplex S.

In order to define an appropriate polyhedron P we begin by remarking that assumption 4.4. implies that the set of non-negative x for which $f(x) \le c$, is bounded. For if there were

a sequence $x^1, x^2...$ tending to infinity with $f(x^j) \le c$, then any limit point of the sequence

$$(x^{j}/||x^{j}||)$$

would be non-negative, different from zero and map into a vector all of whose coordinates were less than or equal to 0. For specificity let us assume that there is a positive constant M, such that $x \geq 0$, and f(x) < c implies that

4.5. [Definition] The polyhedron P is defined to be the product of the closed unit interval $0 \le x_{n+1} \le 1$ with the set $\{(x_1,\dots,x_n) \mid x_i \ge 0, \sum\limits_{1}^{\Sigma} x_i \le M\}$. Each piece P_i is determined by a particular simplex of the subdivision, S_i , and consists of all (x_1,\dots,x_n,x_{n+1}) with

1.
$$0 \le x_{n+1} \le 1$$

2.
$$\sum_{i=1}^{n} x_{i} \leq M \quad , \qquad \text{and} \quad$$

3.
$$(x_1,...,x_n) / \sum_{i=1}^{n} x_i$$
 contained in S_i .

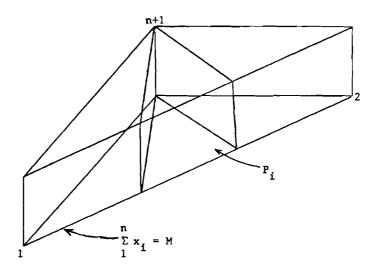


Figure 19.

We also define the function $F(\mathbf{x}_1,\dots,\mathbf{x}_n,\mathbf{x}_{n+1})$ in the following way.

4.6. [Definition] Let d be a vector in R^n which is strictly larger than c, and assume--for definiteness--that

$$\frac{c_j}{d_j} > \frac{c_1}{d_1} \quad \text{for } j = 2, \dots, n \quad .$$

We then define

$$f(x_1,...,x_n,x_{n+1}) = f(x_1,...,x_n + x_{n+1}d$$
.

With this definition a solution to the vector labelling problem will be obtained by finding a vector $(\mathbf{x}_1,\dots,\mathbf{x}_n,\mathbf{x}_{n+1})$ in $\mathbf{F}^{-1}(\mathbf{c})$ with $\mathbf{x}_{n+1}=0$. In order to argue that such a vector does indeed exist let us examine the intersection of $\mathbf{F}^{-1}(\mathbf{c})$ with those boundary faces of P other than that face with $\mathbf{x}_{n+1}=0$.

1. The upper face $x_{n+1} = 1$.

An intersection on this face would satisfy $f(x_1,...,x_n) + d = c$, which is ruled out by sssumption 4.4. since d > c.

2. The face $\sum_{i=1}^{n} x_{i} = M, x_{n+1} > 0.$

Such an intersection would satisfy $f(x_1, ..., x_n) < c$ and n $\sum x_i = M$, which is again impossible by the implications of 1 assumption 4.4.

3. The face $x_i = 0$, for i = 1, ..., n.

On any such face the function f(x) is the identity, and the system of equations F(x) = c may therefore be written as $x + dx_{n+1} = c$ or

$$x = c - dx_{n+1} .$$

Given our assumption however that $c_1/d_1 < c_j/d_j$ for j = 2,...,n, it is easy to see that the only such intersection is the vector $x^* = (c - (c_1/d_1)d,c_1/d_1)$, on the face $x_1 = 0$.

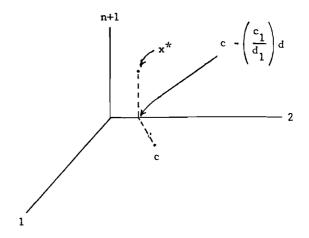


Figure 20.

We have reached the important conclusion that $F^{-1}(c)$ intersects the boundary of P, other than that part of boundary where $x_{n+1}=0$, in a <u>single</u> point. If c is a regular value of the mapping this completes our argument, since the path beginning at x^* must reach a second boundary point of P which necessarily lies in the face $x_{n+1}=0$. If c is not a regular value of the mapping we appeal to Theorem 5.3. The image of the face $x_1=0$, under F, is clearly of dimension n (since f is the identity on that face) and we therefore conclude that there are values of x', lying on that same face and arbitrarily close to x^* , for which c'=F(x') is regular. The system of equations f(x)=c' will therefore have solutions, and by passing to the limit, so will the original system.

It may be useful, as a final remark, to show that the path generated above--when c is a regular value--moves through a sequence of simplices which is identical to that generated by the algorithm described in Scarf and Hansen [22]. Consider two adjacent pieces of linearity P_1 and P_2 whose commong face Q is traversed by the path. Since c is a regular value the

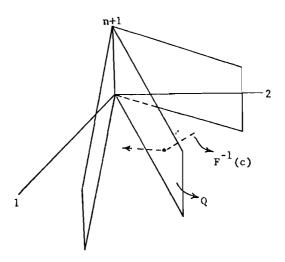


Figure 21.

mapping F must take Q into a subset of \mathbb{R}^n of full dimension, for otherwise a component of $\mathbb{F}^{-1}(c)$ would be fully in this face.

Let us express the action of F on Q as follows. The piece P_1 is generated by a simplex in the subdivision with vertices $v_1^j, v_2^j, \dots, v_n^j$ and P_2 by the simplex, say, in which v_n^j is replaced by v_n^j . Any $(x_1, \dots, x_n, x_{n+1})$ on the face Q can therefore be written as

$$(x_1, ..., x_n) = \alpha_{j_2} v^{j_2} + ... + \alpha_{j_n} v^{j_n}$$
, so that
$$F(x_1, ..., x_n, x_{n+1}) = \alpha_{j_2} f(v^{j_2}) + ... + \alpha_{j_n} f(v^{j_n}) + x_{n+1} d$$

Since this mapping has full rank, it follows that the matrix

$$A = \begin{bmatrix} d_1 & f_1(v^{j_2}) \dots f_1(v^{j_n}) \\ \vdots & \vdots & \ddots & \vdots \\ d_n & f_n(v^{j_2}) \dots f_n(v^{j_n}) \end{bmatrix}$$

has a non-singular determinant. Since $A(x_{n+1}, \alpha_{j_2}, \dots, \alpha_{j_n})' = c$ at the point of intersection of the path and Q, it follows that the columns of A form a feasible basis whose columns correspond to the vertices of the simplex defining P_1 —with the single exception that the column d has replace the image $f(v^{-1})$. This is precisely the general position of the conventional almost complementary algorithm.

The paper continues with several other examples and a discussion of the index of a solution.

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Analysis of a Compact Predator-Prey Model The Basic Equations and Behaviour

Dixon D. Jones

Introduction

This paper is the first of a series dealing with the analysis of a compact, relatively uncomplicated predator-prey model.

Here, only the basic equations are given and a selected subset of system behaviour illustrated. Written documentation concerning this model and its analytic investigation are being documented as completed to speed communication among interested parties. As this model is becoming a focus for several methodological and conceptual discussions, the need has arisen for a concise description of the equations.

The model itself stands midway between more traditional differential or difference equation systems and complex simulation models. (For a review of systems of the former type and access to the flavor of their behaviour, see May, 1973 or Maynard Smith, 1974.) This model is not an embellishment of simpler classic equations but rather an aggregation and consolidation of a complex detailed predator-prey simulation model developed from an extensive program of experiment and submodel development (Holling, 1965, 1966a, Griffiths and Holling, 1969). The objectives of that program are best summarized in Holling 1966b. The complete model continues to be refined, but a detailed documentation, with primary emphasis on the predation process has been prepared (Holling, 1973b). In its present form the

model is a synthesis of the best validated components of the analog processes of predation and parasitism.

The performance of the simulation model exhibits dynamic systems behaviour with far-reaching conceptual and theoretical implications. Holling's paper (1973a) on the resilience of ecological systems is the overture to a major reorientation of ecological perspective. To further explore the dynamic properties of this class of system, we mathematically and pragmatically require an analytic system that is tractable while providing the rich variety of behaviour found in the full simulator.

The goal of this series of IIASA working papers is to explore the dynamic topology of this analytic system and outline a general protocol for analysis of similar systems. There is clearly room to venture back into the ecological domain and use this model to gain insight into the biological aspects of the predation process. However, such a move is not envisioned in the current context. In a subsequent paper I will include a discussion of the theoretical and experimental foundations of this model complete with ecological assumptions and limitations. At present I am offering a system of equations for mathematical enquiry.

The Model Equations

The model is equivalent to a deterministic pair of difference equations. Indeed it can be so formulated, but to do that would cloud, rather than clarify. The iteration time interval is unspecified in absolute terms. During each time step, predators

attack and remove prey. Then predators and prey both reproduce. The event orientation of the formulation ties the iteration most strongly to the prey generation time.

The two state variables are the densities of predators and of prey. At the start of each iteration the initial densities are

The functional response of predator attacks to prey density is

$$g(x) = \frac{a_1 x e^{\alpha x}}{1 + a_2 x e^{\alpha x}} = \frac{a_1 x}{e^{-\alpha x} + a_2 x}$$
 (2)

Because attacks of predators on prey are distributed nonrandomly among the prey, we incorporate the negative binomial distribution to account for this (see Griffiths and Holling, 1969). The number (per unit area) of prey attacked is z and is expressed as

$$z = f(x,y) = x \left\{ 1 - 1 \left[+ \frac{k_1 \cdot y \cdot g(x)}{kx} \right]^{-k} \right\} . \tag{3}$$

The number of prey that excape predation is

$$\hat{x} = x - z . \tag{4}$$

These reproduce according to some function $H(\hat{x})$ that provides

a density of prey x' at the beginning of the next time step.

The reproduction function used is a descriptive one. It incorporates a minimum density reproduction threshold and a maximum at some finite prey density.

Prey reproduction depends on three parameters:

$$x_{O}$$
 = minimum density for reproduction
$$M = maximum reproductive rate$$
 OPTX = prey density at maximum reproduction rate (5)

These parameters are recombined as

$$\gamma = 1 + OPTX$$

$$\mu = OPTX - x_O = \gamma - 1 - x_O$$

$$CH = \frac{M \cdot e^{\mu}}{\mu} = M(\frac{e}{\mu})^{\mu} = M \cdot C_{\mu} . \qquad (6)$$

The final form of $H(\hat{x})$ is

$$\mathbf{x'} = \mathbf{H}(\hat{\mathbf{x}}) = \mathbf{C}\mathbf{H} \cdot \mathbf{e}^{-(\hat{\mathbf{x}} - \mathbf{x}_0)} \cdot (\hat{\mathbf{x}} - \mathbf{x}_0)^{\mu} \cdot \hat{\mathbf{x}}$$
 (7)

The function describing predator reproduction incorporates both "contest" and "scramble" types (Nicholson, 1954). The parameter C, varies between 0 and 1, and specifies the degree of scramble in the process. The predator density that begins the next iteration, y', is given as

$$y' = p(x,z) = c_1 \cdot z \left(1 - C \cdot z \frac{1+k}{k \cdot x + z}\right)$$
 (8)

In summary the equations are

$$g(x) = \frac{a_1 x}{e^{-\alpha x} + a_2 x}$$
 (2)

$$z = f(x,y) = x \cdot 1 - 1 + \frac{k_1 \cdot y \cdot g(x) - k}{kx}$$
 (3)

$$\hat{x} = x - z \tag{4}$$

$$x' = H(\hat{x}) = CH \cdot e^{-(\hat{x}-x_0)} \cdot (\hat{x} - x_0)^{\mu} \cdot \hat{x}$$
 (7)

$$y' = p(x,z) = c_1 z - 1 - C \cdot z \frac{1+k}{k \cdot x + z}$$
 (8)

The "graph" of this model is relatively simple (Figure 1). The quantity y' is entered twice to emphasize the symmetry. The broken arrows from x' to x and from y' to y indicate a new iteration in the time sequence.

Model Behaviour

A BASIC program was written to implement this model on a Hewlett-Packard 9830A calculator. A small subset of the possible conditions are illustrated in Figures 2 through 5.

In the course of development of this experimental and modelling work, certain parameters have evolved into what we call our "Standard Case". These particular values do not necessarily carry any fundamental biological significance; they only serve as a common base for comparing the effect of changes in parameter values. The "Standard Case" in the present notation is

 $a_1 = 2.5$

 $a_2 = 0.0714$

 $\alpha = 0$

 $k_1 = 30$

k = 0.78

 $x_0 = 0.001$

 $\gamma = 1.1$

M = 3.0

C = 0

 $c_1 = 0.95$

Note: In the figures that follow a value of $a_2 = 0.0714$ was inadvertently used. The resulting differences are minor.

Figure 2 shows a phase plane trajectory for the Standard Case. The initial starting point is at "x"; the trajectory then spirals counter-clockwise into an equilibrium point. (The trajectory has been terminated before it reached that point.)

The Standard Case is not globally stable. Combinations of state variables that lead to prey densities less than x_{0} result in extinction of the prey population followed by the predators. Figure 3 shows an enlarged section of the state plane with a disperse collection of starting conditions. The actual trajectories have been suppressed in this plot. Initial points are marked with "x"; subsequent locations are marked with "O" if they are outside the domain of attraction or with "+" if they eventually lead to equilibrium. With enough trial initial points, the boundary of the attractor domain begins to be defined as indicated by the freehand curve.

Previous explorations with the full simulation model have identified K and C as important and sensitive parameters to the topology of trajectories (Jones, 1973). Table I. outlines the qualitative behaviour trends for increasing values of k for C = 0 ("contest" predator reproduction) and C = 1 ("scramble" reproduction). The exact division between these models have not been located. They could be, of course, given enough paper and patience. The goal of the present analytic effort is to shortcut that necessity and develop a more comprehensive procedure for looking at this type of system.

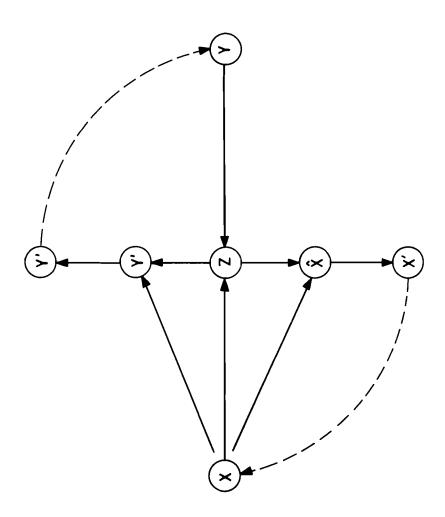
As one example of the behaviour of this model see Figures 4 and 5 in conjunction with Figure 2. When the binomial coefficient k = 1.0 the system becomes globally unstable (Fig. 4). The analogy of Hopf bifurcation would suggest that there is an intermediate range of k values for which a periodic orbit exists. Figure 5 shows the phase behaviour for k = 0.825. A periodic orbit does seem possible although visual inspection is not an absolute judge.

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Table I. Behaviour trend with increasing k, for C = 0 and C = 1.

k	C = 0	C = 1	k
0	Long Narrow Domain of Attraction (perhaps extending to $y = \infty$)		0
~ 0.4 0.6	Beginning of Oscillatory Trajectories. Finite Domain.	Large Domain of Attraction (perhaps infinite in high x, y corner)	
0.825	Neutral Orbits Inside a Finite Domain		
	Global Instability Increasing speed to extinction.		· .
		Finite Domain of Attraction Contraction of Domain	10
			100



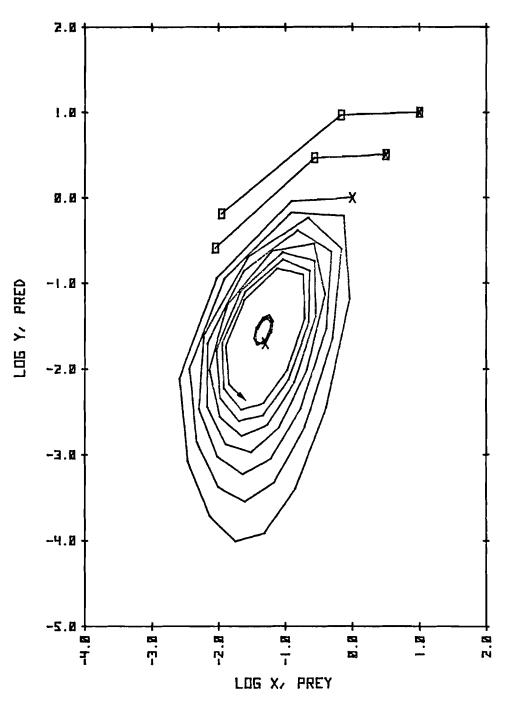


Figure 2. Sample Trajectories for "Standard Case"

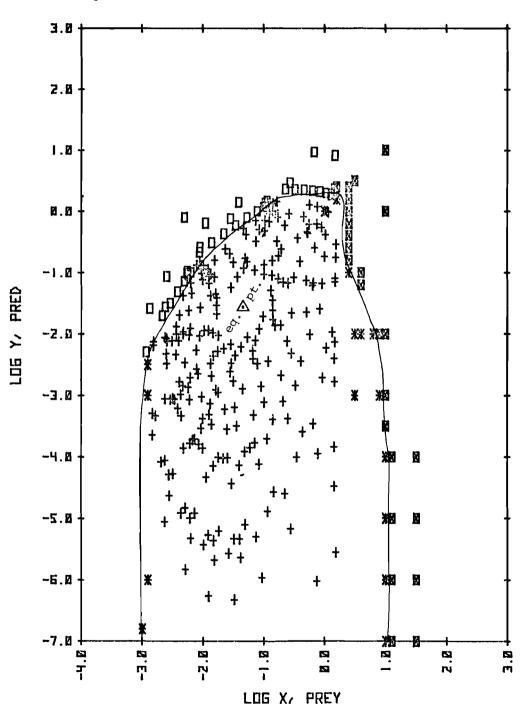


Figure 3. Domain of Attraction for "Standard Case"

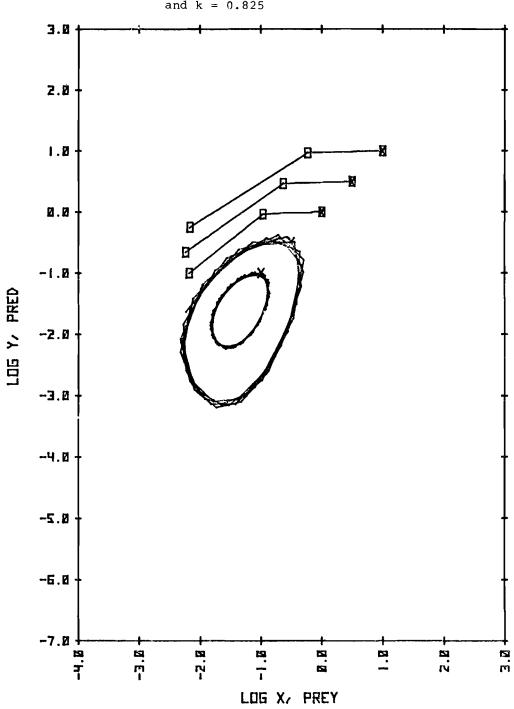


Figure 5. Sample Phase Plane Trajectory for C=0 and k=0.825

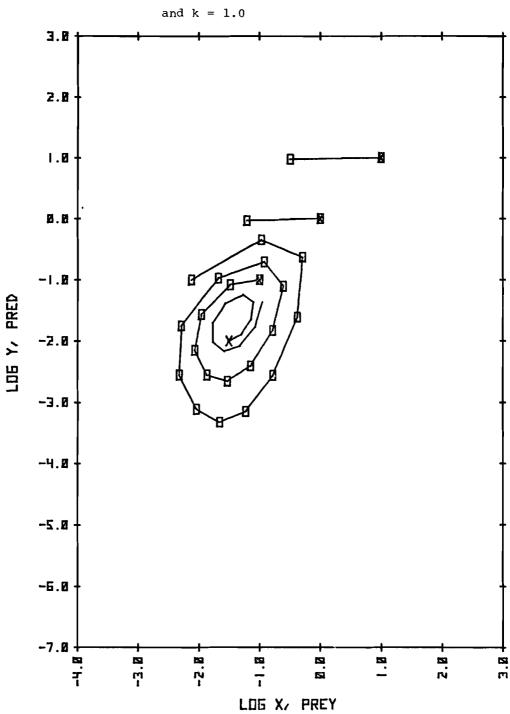


Figure 6. Sample Phase Plane Trajectory for C = 0

Volterra's System and the Equation of Michaelis-Menten

A.D. Bazykin

Abstract of presentation

A modified set of Volterra's differential equations for dynamics of prey and predator population sizes is analyzed. This modification takes three effects into consideration:

- 1) Satiation of predator resulting in the incapacity of both the rate of eating away of prey by predator and the rate of predator reproduction to increase infinitely with growth of prey number.
- 2) Limited resources of prey, as a result of which prey population size cannot increase infinitely even in the absence of predator.
- 3) Limited external resources (unrelated to prey) of predator, as a result of which predator population size cannot grow infinitely even when there is an excess of preys:

$$\dot{x} = ax - \frac{bxy}{1 + \alpha x} - \varepsilon x^2$$

$$\dot{y} = -cy + \frac{dxy}{1 + \alpha x} - \mu y^2$$

Analysis of this set of equations gives many different regimes depending on the values of parameters.

This model as a whole prognoses a number of situations: situations in which the behavior of a predator-prey system is adequately described by Volterra's equations; situations in

which these equations cannot describe the dynamics of preypredator relations; situations in which these relations change similarily to Volterra's under certain initial conditions and does not change in other conditions.

Stability Analysis of Predator-Prey Models

Via the Liapunov Method*

M. Gatto and S. Rinaldi*

Abstract

As is well known from the classical applications in the electrical and mechanical sciences, energy is a suitable Liapunov function; thus, by analogy, all energy functions proposed in ecology are potential Liapunov In this paper, a generalized Lotka-Volterra functions. model is considered and the stability properties of its non-trivial equilibrium are studied by means of an energy function first proposed by Volterra in the context of conservative ecosystems. The advantage of this Liapunov function with respect to the one that can be induced through linearization is also illustrated.

1. Introduction

One of the classical problems in mathematical ecology is the stability analysis of equilibria and, in particular, the determination of the region of attraction associated with any asymptotically stable equilibrium point. It is also known that the best way of obtaining an approximation of such regions is La Salle's extension of the Liapunov method [2], [4].

Nevertheless, this approach has not been very popular among ecologists, the main reason being that Liapunov functions (i.e. functions that satisfy the conditions of the Liapunov method) are in general difficult to devise. One straightforward, but often not very effective, way of overcoming this difficulty is through linearization as shown in Section 3, while a more fruitful

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way consists in considering as candidates for Liapunov functions any functions that are analogous to the internal energy of the system. This is the approach that is, for example, commonly followed by engineers in the analysis of mechanical systems or in the study of nonlinear electrical networks. The reason why the Liapunov method has not been widely used in ecology possibly resides in the lack of a definition of an energy function in the context of ecological systems. One major exception is represented by the pioneering work of Volterra and the more recent work of Kerner [1] who discussed the analogy between ecological and mechanical systems in terms of energy. Nevertheless, these works are limited to conservative ecosystems, a case that seems to be very peculiar indeed.

The aim of this paper is to show how the energy function proposed by Volterra (from now on called Volterra function) quite often turns out to be a Liapunov function even for non-conservative ecosystems. In order to avoid complexity in notation and proofs, the only case that is dealt with in the following is the one of second order (predator-prey) systems, but the authors strongly conjecture that the results presented in this paper could be easily generalized to more complex ecological models.

2. The Volterra Function

Consider the simple Lotka-Volterra model

$$\frac{\mathrm{dx}}{\mathrm{dt}} = \mathbf{x}(\mathbf{a} - \mathbf{by}) \tag{1.a}$$

$$\frac{dy}{dt} = y(-c + dx) \tag{1.b}$$

where x and y are prey and predator populations and (a,b,c,d) are strictly positive constants. This system has a non-trivial equilibrium $(\overline{x},\overline{y})$ given by $(\overline{x},\overline{y})=(c/d,a/b)$ which is simply stable in the sense of Liapunov. Moreover, any initial state in the positive quadrant gives rise to a periodic motion. This can easily be proved by means of the energy function proposed by Volterra,

$$V = (x/\overline{y} - \log x/\overline{x}) + p(y/\overline{y} - \log y/\overline{y}) - (1 + p) , (2)$$

where

$$p = b\overline{y}/d\overline{x}$$
,

since this function is constant along any trajectory and its contour lines are closed lines in the positive quadrant. In other words, the Volterra function (2) is a Liapunov function because it is positive definite and its derivative dV/dt is negative semidefinite (identically zero).

In the following, the Volterra function will be used in relation with non-conservative ecosystems of the form:

$$\frac{dx}{dt} = x(a - by + f(x,y))$$

$$\frac{dy}{dt} = y(-c + dx + g(x,y)) ,$$
(3)

where f and g are continuously differentiable functions. Moreover, we assume that there exists a non-trivial equilibrium $(\overline{x},\overline{y}) > 0$ and that the positive quadrant is an invariant set for system (3) so that it can be identified from now on with the state set of the system.

3. Linearization and the Liapunov_Equation

Liapunov functions can, of course, be constructed by solving the so-called Liapunov equation. This procedure is now briefly described so that the advantage of the Volterra function can be better appreciated in the next sections. Let

$$\delta \mathbf{x} = \mathbf{x} - \overline{\mathbf{x}}$$

$$\delta y = y - \overline{y}$$

be the variations of prey and predator populations with respect to the equilibrium $(\overline{x},\overline{y})$. Then the linearized system associated with this equilibrium is given by

$$\frac{d}{dt} \begin{bmatrix} \delta x \\ \delta y \end{bmatrix} = F \begin{bmatrix} \delta x \\ \delta y \end{bmatrix} = \begin{bmatrix} \overline{f}_{x} \overline{x} & (-b + \overline{f}_{y}) \overline{x} \\ (d + \overline{g}_{x}) \overline{y} & g_{y} \overline{y} \end{bmatrix} \begin{bmatrix} \delta x \\ \delta y \end{bmatrix} , \quad (4)$$

where $(\overline{f}_x, \overline{f}_y, \overline{g}_x, \overline{g}_y)$ are the partial derivatives of f and g evaluated for $(x,y) = (\overline{x}, \overline{y})$. Now, assume that the matrix F has eigenvalues with negative real parts, which implies that the

equilibrium is asymptotically stable (recall that the converse is not true). Under this assumption Liapunov's equation (matrix equation)

$$\mathbf{F}^{\mathbf{T}}\mathbf{P} + \mathbf{P}\mathbf{F} = -\mathbf{Q} \tag{5}$$

has one and only one solution in the unknown matrix P for any positive definite matrix Q. Moreover, the matrix P is positive definite and the function

$$W = \left| \delta \mathbf{x} \quad \delta \mathbf{y} \right| \mathbf{P} \left| \delta \mathbf{x} \quad \delta \mathbf{y} \right|^{\mathbf{T}} \tag{6}$$

is a Liapunov function because its derivative

$$\frac{dW}{dt} = - \left| \delta \mathbf{x} \quad \delta \mathbf{y} \right| Q \left| \delta \mathbf{x} \quad \delta \mathbf{y} \right|^{T}$$

is negative definite. In conclusion, the Liapunov function (6) can be very easily determined by solving equation (5) with F given as in equation (4) and with Q positive definite (e.g. Q = indentity matrix). The only limitation to the applicability of this method is the assumption on the eigenvalues of the matrix F: for example, the Lotka-Volterra model (1) cannot be discussed in this way, since the F matrix has purely imaginary eigenvalues. Nevertheless, even when this method can be applied, the results are not in general as satisfactory as the ones that can be obtained by means of the Volterra function as shown in the next section.

4. The Volterra Function as a Liapunov Function

Consider the generalized Lotka-Volterra model (3) and the Volterra function V given by equation (2). Then, the derivative of the Volterra function along trajectories is given by

$$\frac{dV}{dt} = \frac{\partial V}{\partial x} \frac{dx}{dt} + \frac{\partial V}{\partial y} \frac{dy}{dt} = \left(\frac{x}{x}\right) - 1 \left(a - by + f(x,y)\right)$$
$$+ \frac{b\overline{y}}{d\overline{x}} \left(\frac{y}{\overline{y}} - 1\right) \left(-c + dx + g(x,y)\right)$$

In order to study dV/dt in a neighborhood of the equilibrium $(\overline{x},\overline{y})$, it is possible to expand this function in Taylor series up to the second order terms, i.e.,

$$\frac{dV}{dt} \simeq \frac{dV}{dt}\Big|_{\overline{x},\overline{y}} + \frac{d}{dx}\left(\frac{dV}{dt}\right)\Big|_{\overline{x},\overline{y}} \delta x + \frac{d}{dy}\left(\frac{dV}{dt}\right)\Big|_{\overline{x},\overline{y}} \delta y$$

$$+ \frac{1}{2} \frac{d^{2}}{dx^{2}} \left(\frac{dV}{dt}\right)\Big|_{\overline{x},\overline{y}} (\delta x)^{2} + \frac{1}{2} \frac{d^{2}}{dy^{2}} \left(\frac{dV}{dt}\right)\Big|_{\overline{x},\overline{y}} (\delta y)^{2}$$

$$+ \frac{d^{2}}{dxdy} \left(\frac{dV}{dt}\right)\Big|_{\overline{x},\overline{y}} \delta x \delta y \quad . \tag{7}$$

Since

$$\frac{d\mathbf{v}}{d\mathbf{t}}\Big|_{\overline{\mathbf{x}}, \overline{\mathbf{y}}} = \frac{d}{d\mathbf{x}} \left(\frac{d\mathbf{v}}{d\mathbf{t}} \right) \Big|_{\overline{\mathbf{x}}, \overline{\mathbf{y}}} = \frac{d}{d\overline{\mathbf{y}}} \left(\frac{d\mathbf{v}}{d\mathbf{t}} \right) \Big|_{\overline{\mathbf{x}}, \overline{\mathbf{y}}} = 0$$

$$\frac{d^2}{dx^2} \left(\frac{dV}{dt} \right) \Big|_{\overline{x}, \overline{y}} = \frac{2\overline{f}_x}{\overline{x}}$$

$$\frac{d^2}{dy^2} \left(\frac{dV}{dt} \right) \Big|_{\overline{x}, \overline{y}} = \frac{2b\overline{g}_y}{d\overline{x}}$$

$$\frac{d^2}{dxdy} \left(\frac{dV}{dt} \right) \Big|_{\overline{x}, \overline{y}} = \frac{\overline{f}_y}{\overline{x}} + \frac{b\overline{g}_x}{d\overline{x}} ,$$

eq. (7) becomes

$$\frac{dV}{dt} \simeq \frac{1}{2} [\delta \mathbf{x} \ \delta \mathbf{y}] \begin{bmatrix}
\frac{2\overline{f}_{\mathbf{x}}}{\overline{\mathbf{x}}} & \frac{\overline{f}_{\mathbf{y}}}{2\overline{\mathbf{x}}} + \frac{b\overline{g}_{\mathbf{x}}}{2d\overline{\mathbf{x}}} \\
\frac{\overline{f}_{\mathbf{y}}}{2\overline{\mathbf{x}}} + \frac{b\overline{g}_{\mathbf{x}}}{ad\overline{\mathbf{x}}} & \frac{2b\overline{g}_{\mathbf{y}}}{d\overline{\mathbf{x}}}
\end{bmatrix} [\delta \mathbf{x} \ \delta \mathbf{y}] . \tag{8}$$

Therefore the second order approximation of dV/dt turns out to be a homogeneous quadratic form; by studying the negative or positive definiteness of such a form, it is possible to derive sufficient conditions for the Volterra function to be a Liapunov function. More precisely, by applying the well-known Sylvester conditions and performing easy computations, we obtain

$$\left. \begin{array}{c} \overline{f}_{x} < 0 \\ b\overline{g}_{x} + d\overline{f}_{y} < 4bd\overline{f}_{x}\overline{g}_{y} \end{array} \right\} \frac{dV}{dt} \text{ negative definite} \tag{9}$$

$$\left. \begin{array}{c} \overline{f}_{x} > 0 \\ b\overline{g}_{x} + d\overline{f}_{y} \end{array} \right\} \xrightarrow{2} + 4bd\overline{f}_{x}\overline{g}_{y} \qquad \qquad (10)$$

Notice that these conditions are only sufficient for Liapunov methods to be applicable; thus, even if these conditions are not satisfied, it is possible that the Volterra function turns out to be a Liapunov function (see Example 2).

As far as the study of stability properties in the large is concerned, the Volterra function is definitely advantageous with respect to the quadratic forms derived by means of Liapunov's equation (5). This is apparent in the case of global stability; in fact, global stability can be inferred by means of Volterra function, whose contour lines in the state set are closed, while this is never possible by means of a positive definite quadratic form of the kind (6), since the contour lines are not closed (see Examples 1 and 2).

5. Examples

This section is devoted to clarifying by means of some examples what has been discussed above, with particular emphasis on the trade-offs between the Volterra function and the quadratic Liapunov function that can be obtained by solving the Liapunov equation.

Example 1

The first example is a simple symmetric competition model for two species described by the following equations (see May [3]:

$$\frac{dx}{dt} = x(k_1 - x - \alpha y)$$

$$\frac{dy}{dt} = y(k_2 - y - \alpha x) ,$$

where $\boldsymbol{k}_{1},~\boldsymbol{k}_{2}$ and $\boldsymbol{\alpha}$ are positive parameters.

Provided that

$$\begin{cases} \alpha k_2 > k_1 \\ \alpha k_1 > k_2 \end{cases} \begin{cases} \alpha k_2 < k_1 \\ \alpha k_1 < k_2 \end{cases}$$

a non-trivial equilibrium $(\overline{x},\overline{y})$ exists and is given by

$$(\overline{x},\overline{y}) = \left(\frac{\alpha k_2 - k_1}{\alpha^2 - 1}, \frac{\alpha k_1 - k_2}{\alpha^2 - 1}\right).$$

Thus, the matrix F of the linearized system is given by

$$\mathbf{F} = \begin{bmatrix} -\overline{\mathbf{x}} & -\alpha \overline{\mathbf{x}} \\ \\ -\alpha \overline{\mathbf{y}} & -\overline{\mathbf{y}} \end{bmatrix}$$

and its eigenvalues have negative real parts, provided that its trace is strictly negative and its determinant is strictly positive. These conditions are obviously satisfied if α < 1. On the other hand, also the sufficient conditions given by eq. (9) work well. In fact

$$\overline{f}_{v} = -1 < 0$$

and

$$(b\overline{g}_{x} + d\overline{f}_{y})^{2} = \alpha^{2}(1 + \alpha)^{2} < 4bdf_{x}\overline{g}_{x} = 4\alpha$$

provided that $\alpha < 1$.

However, the Volterra function guarantees the global stability of the equilibrium. This can be easily understood when taking into account that there is no error in the Taylor expansion (7), because the functions f and g are linear. Thus, dV/dt is negative definite in the state set and global stability follows from La Salle's conditions.

Example 2

Consider the well-known modification obtained from the classical Lotka-Volterra model, when assuming, in the absence of predation, a logistic growth for the prey:

$$\frac{dx}{dt} = x(a - by - kx)$$

$$k > 0 .$$

$$\frac{dy}{dt} = y(-c + dx)$$

If ad > kc a non-trivial equilibrium

$$(\overline{x},\overline{y}) = \left(\frac{c}{d}, \frac{a}{b} - \frac{kc}{bd}\right)$$

exists, and linearization around it yields

$$F = \begin{bmatrix} -\frac{kc}{d} & -\frac{bc}{d} \\ \\ \frac{da - kc}{b} & 0 \end{bmatrix}$$

which has eigenvalues with negative real parts. On the other hand, it turns out that

$$\overline{f}_{x} = -k$$

$$4bd\overline{f}_{x}\overline{g}_{x} = (b\overline{g}_{x} + d\overline{f}_{y})^{2} = 0$$
.

Therefore eq. (9) is not satisfied. Nevertheless, a direct computation yields

$$\frac{dV}{dt} = -\frac{k}{b\overline{x}\overline{y}} (x-\overline{x})^2 ,$$

i.e. dV/dt is negative semidefinite. Since the locus dV/dt = 0 is not a trajectory of the system (easy to check), Krasowskyi conditions are met with and asymptotic stability can be inferred. Moreover, since dV/dt is negative semidefinite in the whole state set, global stability can be straightforwardly deduced.

Example 3

A third example is given to show how a subregion of the region of asymptotic stability can be found by means of the Volterra function.

Consider a situation where the prey, in the absence of predators, has an asymptotic carrying capacity β and a minimum density α , below which successful mating cannot overcome the death process. This model can be described by

$$\frac{dx}{dt} = x(-(x - \alpha)(x - \beta) - \gamma y)$$

$$\frac{dy}{dt} = y(-c + x)$$

where $\alpha,\ \beta,\ \gamma$ are positive parameters which are supposed to satisfy the relations

$$a < c < \beta$$

$$\frac{\alpha + \beta}{2} < c .$$

It is easy to check that there exists only one non-trivial equilibrium given by $(\overline{x}, \overline{y}) = \left(c, -\frac{(c-\alpha)(c-\beta)}{\gamma}\right)$.

This equilibrium is not globally stable, since the origin of the state space is also asymptotically stable. The regions A and B of asymptotic stability obtained by simulation for particular values of the parameters are shown in Figure 1. It

is possible to determine an approximation of region A by means of the Volterra function. In fact,

$$\frac{dV}{dt} = \left(\frac{x}{\overline{x}} - 1\right) \left(-(x - \alpha)(x - \beta) - \gamma y\right) + \gamma \frac{\overline{y}}{\overline{y}} \left(\frac{y}{\overline{y}} - 1\right) \left(-c + x\right)$$

$$= \frac{1}{\overline{x}} (x - \overline{x})^{2} (\alpha + \beta - c - x)$$

is negative semidefinite in the region

$$x > a + \beta - c$$

since $(\alpha + \beta)/2 < c$. Moreover the straight line $x = \overline{x}$, where dV/dt = 0, does not contain any perturbed trajectory. Therefore the region bounded by the contour line of the Volterra function that is tangent to the straight line $x = \alpha + \beta - c$ (see Figure 1) represents an estimate of the region of attraction, since La Salle's conditions are satisfied.

6. Concluding Remarks

The energy function proposed by Volterra has been used in this paper to analyze the asymptotic behavior of non-conservative ecosystems of the predator-prey type. The main result is that the Volterra function turns out to be a well-defined Liapunov function for a large class of systems and therefore allows the discussion of the local and global stability properties of such

systems. The Volterra function definitely seems advantageous with respect to the Liapunov functions that can be obtained through linearization, particularly in the case of global stability. Moreover, it is worthwhile noting that the Volterra function is also of interest when the equilibrium state under discussion is unstable. The results obtained in this paper allow us to prove in a very simple form some general properties such as the following: if the function f and g in the general model (3) are linear and satisfy eq. (9), then the local stability of an equilibrium implies its global stability.

Acknowledgement

The authors are grateful to Dr. Dixon D. Jones for his helpful suggestions and advice.

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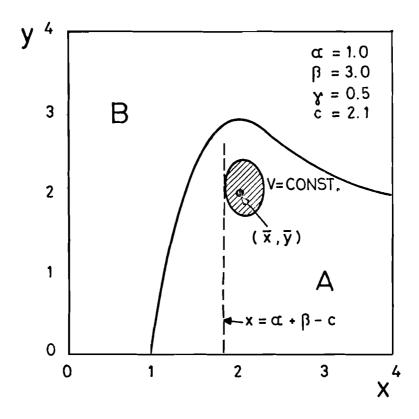


Figure 1. The estimation of the region A of attraction by means of the Volterra function.

J. Casti (presented July 28)

I. Introduction

The basic question to be studied in this presentation is the determination of the boundary of stability (domain of attraction) of the origin for the system

$$\dot{x}(t) = f(x)$$
 , $x(0) = x_0$, $t \ge 0$. (*)

Here x(t) is an n-dimensional vector function of time and f is a continuous vector-valued function of x such that f(0) = 0.

The Zubov procedures for determining the domain of attraction are based on

Theorem 1[1]. In order that the region $A \subset E^n$, containing the origin, be the domain of asymptotic stability for the zero solution of (*), it is necessary and sufficient that there exist functions V(x) and $\phi(x)$ such that

- 1) the function V(x) is continuous in A, while $\phi(x)$ is continuous in E^n ;
 - 2) -1 < V(x) < 0 for $x \in A$, $\phi(x) > 0$ for $x \in E^n$, $|x| \neq 0$;
- 3) for any $\gamma_2 > 0$, we can find γ_1 and α_1 such that $V(x) < -\gamma_1 \text{ for } |x| \ge \gamma_2, \ \phi(|x|) > \alpha_1 \text{ for } |x| \ge \gamma_2;$
 - 4) V(x) and $\phi(x) \rightarrow 0$ as $|x| \rightarrow 0$;
 - 5) if $y \in \partial A$, $y \neq 0$, then $\lim_{x \to y} V(x) = -1$, while if

 $|x| \rightarrow + \infty$, $x \in A$, then $V(x) \rightarrow -1$;

6)
$$\left[\frac{dV}{dt}\right] = \phi(x) (1 + V(x)) \left[1 + \sum_{i=1}^{n} f_i^2\right]^{1/2}$$
.

An important corollary of Theorem 1, valid for f continuouslydifferentiable in each argument is

Corollary 1. If the zero solution of (*) is asymptotically
stable, then the equation

$$\sum_{i=1}^{n} \frac{\partial V}{\partial x_i} f_i(x_1, \dots, x_n) = \phi(x_1, \dots, x_n) (1 + V(x)) \begin{bmatrix} 1 + \sum_{i=1}^{n} f_i^2 \end{bmatrix}^{1/2} \quad (**)$$

has a unique continuously differentiable solution defined by the condition V(0) = 0, for all xeA, satisfying the conditions of Theorem 1 for some function ϕ . In order that (**) have a solution it suffices that ϕ satisfy

$$\int_{0}^{\infty} \phi(x) dt < \infty$$

for sufficiently small x_0 .

(Remark: The reader should note that the conditions of Theorem 1 make $V(\vec{x})$ a Lyapunov function for (*)).

Example:

$$\dot{x} = -x + 2x^2y$$

The equation for V is

$$\frac{\partial V}{\partial x}(2x^2y - x) + \frac{\partial V}{\partial y}(-y) = (x^2 + y^2)(1 + V) ,$$

which is obtained by choosing

$$\phi(x,y) = \frac{x^2 + y^2}{\left[1 + \sum_{i=1}^{n} f_i^2\right]^{1/2}}.$$

It is easy to see that

$$V(x,y) = \exp \left[-y^2/2 - \frac{x^2}{2(1-xy)}\right] - 1$$

is the solution of this equation. From this function it follows that the curve xy = 1 forms the boundary of the stability domain.

II. Zubov's Approach for Analytic Systems

Henceforth, we impose the following restrictions on the system dynamics:

 (A_1) the functions $f_i(x_1,\ldots,x_n)$ are holomorphic functions of (x_1,\ldots,x_n) having no constant terms, i.e.

$$f_s(x_1,...,x_n) = \sum_{i=1}^{n} p_{si}x_i + \sum_{\substack{n \\ k=1}}^{n} m_k > 1$$

 (A_2) the characteristic roots of the linear part of the dynamics all have negative real parts, i.e. if P = $[p_{ij}]$, then the equation

$$det (P - \lambda I) = 0$$

has roots $\{\lambda_i\}$ all in the left half-plane.

Under (A_1) , (A_2) , it is not hard to show that Eq.(**) has a solution of the form

$$V(x) = v_2(x) + v_3(x) + ... + v_m(x) + ... ,$$
 (+)

where $v_m(x)$ is a homogeneous form of degree m in the variables (x_1,\ldots,x_n) . Substituting this representation into Equation (**), we obtain the following recursive equations for the forms $\{v_i(x)\}$:

$$\sum_{i=1}^{n} \frac{\partial v_{2}}{\partial x_{i}} \binom{n}{\sum_{k=1}^{n} p_{ik} x_{k}} = \phi(x_{1}, \dots, x_{n}) ,$$

$$\sum_{i=1}^{n} \frac{v_m}{x_i} \binom{n}{\sum_{k=1}^{n} p_{ik} x_k} = R_m(x_1, \dots, x_n) , \quad m = 3, 4, \dots .$$

Here R is a known form of degree m, determined by knowledge of the forms v_2 , v_3 ,..., v_{m-1} .

The following properties of the series (+) are of special importance:

i) the form $v_2(x)$ is negative definite;

- ii) the series (+) converges in a neighborhood of the origin;
- iii) the function V(x) defined by the convergent series (+), may be analytically continued along any ray emanating from the origins and terminating at the boundary of the domain of stability.

Remark: Choice of the function ϕ influences the region of convergence of (+).

Zubov's attack on the stability problem is based on an attempt to utilize finite segments of the series (+) to successively approximate the stability boundary. The first task is to construct a region entirely contained within the domain of stability.

Consider the family of hypersurfaces $v_2(x) = -\mu$, $0 < \mu < \infty$. Call $\mathscr{S}(= \partial A)$ the true stability boundary. There exists a value of $\mu = \overline{\mu}$ such that the surface $v_2(x) = -\overline{\mu}$ will be tangent to some point of \mathscr{S} . Consequently, since the family $v_2(x) = -\mu$ fills up all of E^n , we let $-\overline{\mu}$ be the largest value of $v_2(x)$ on \mathscr{S} . Then $v_2 = -\overline{\mu}$ will be tangent to \mathscr{S} . Since \mathscr{S} is unknown, we proceed as follows. Let

$$W(x) = \frac{dv_2}{dt} = \sum_{i=1}^{n} \frac{\partial v_2}{\partial x_i} \cdot f_i(x)$$

and find the set of points where W(x) = 0. If we call this set W₀, we now find the largest value of v_2 on W₀ and call this - μ_0 , i.e.

$$-\mu_0 = \max_{x} \{v_2(x) : W(x) = 0\}$$
.

Then we obtain

Theorem 2. The hypersurface $v_2(x) = -\mu_0$ is entirely contained within the domain of attraction of the origin.

The general algorithm proceeds by iterating the above procedure. The steps are:

1) Consider the hypersurfaces $S_n(x) = -\mu$, where $S_n(x) = v_2(x) + \ldots + v_n(x).$ Define

$$W_n(x) = \frac{dS_n}{dt}$$
,

$$W_{0n} = \{x : W_n(x) = 0\}$$
.

- 2) Determine the largest value of \boldsymbol{S}_n on the set $\boldsymbol{W}_{0\,n}.$ Call this value $\boldsymbol{\mu}_{0\,n}.$
- 3) The hypersurface $S_n = -\mu_{0n}$ will then be entirely contained within the domain of attraction. Further, as $n \to \infty$ the regions $S_n = -\mu_{0n}$ will converge to \mathcal{S} .

III. Discussion

Successful use of the Zubov approach hinges critically upon the ability to successfully form the series (+) and to carry out the necessary algebraic manipulations to find the forms $\{v_i(x)\}$. Current symbolic manipulation computer languages such as PL/I, FORMAC, etc. may be helpful in this regard. Also, it should be noted that in many cases all that is required is a

reasonable estimate of the boundary of stability so that it may be possible to use only two or three terms in (+), thereby reducing the computational burden.

Generally speaking, the Zubov procedures are probably not as effective for finding the true domain of stability for an isolated system as the numerical "backward" integration approaches. However, if one is interested in structural features, of the stability boundary and parametric studies, then the Zubov methods are undoubtedly superior as they enable one to systematically generate analytic forms which approximate the boundary of stability to arbitrary accuracy.

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Some Elements of the Response Function of the Enterprise in the Socialist Economy

Janusz Beksiak (presented July 29)

In the analysis of the management system of the national economy we are interested in the vertical relations between central economic authorities (CEA) and enterprises, and horizontal ones between enterprises and consumers. In the empirical research we tried to recognize the ways in which the enterprises respond to the stimuli coming to them from other participants of economic life.

We understand the term "response function" in a very general, informal sense, as a correspondence between information input and output of the enterprise. In our analysis we concentrate on the control elements of this "function", such as: price-type and non-price information and elements of the process of decision-making.

During one year we observed the behavior of some number of the enterprises producing and trading consumer goods. We recorded decisions and events occurring in their behavior.

It is possible to present now in a very short form a part of the provisional results of this work concerning: a) aims, b) decision-making procedure, c) managment instruments and links.

Aims

We selected eight types of aims described by the enterprises:

- 1. Satisfaction of demands of consumers.
- 2. Satisfaction of demands of public opinion.
- 3. Maximization of incomes.
- 4. Minimization of efforts of the personnel.
- Improvement of the enterprise organization and efficiency.
- 6. Satisfaction of demands of other enterprises.
- 7. Satisfaction of demands of central economic activities.*
- Satisfaction of demands of other authorities (political, local, etc.).

These aims occurred in most cases in groups, with one emphasized as the main aim. According to this we selected three aggregated "orientations":

- A. Consumers (combination of the aims 1 and/or 2).
- B. CEA (6, 7, 8).
- C. Own interest (3, 4, 5).

On the basis of frequency of different orientations in the behavior of each enterprise, we divided them into two types:

I oriented on: 1) own interest (C), 2) CEA (B), 3) consumers (A).

II oriented on: 1) consumers (A), 2) own interest (C),
3) CEA (B).

Decision-making procedure

We have taken into account: a) information basis, b) number of variants analyzed, c) method of choice (calculation, notformalized analysis, experience and intuition, routing).

^{*}Other than given in previous items.

After determining the minimum necessary requirements of methodological rationality for different kinds of decisions, we divided them generally into two categories: fully satisfying and not-fully satisfying these requirements. Taking differences from the average figures (average for all analyzed decisions) occurring in each enterprise, we got eight types of decision—making procedures. The greatest number of enterprises belong to types No. 3, 5, and 8 (see Figure).

Management instruments and links

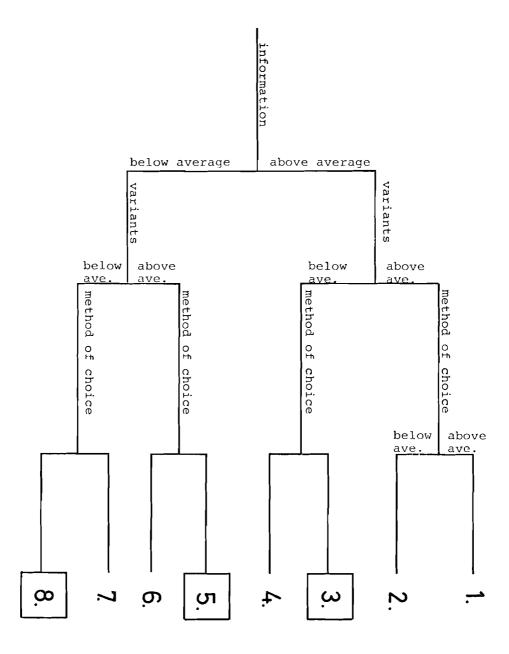
We distinguish

- three groups of instruments: a) directives, b) pricetype instruments, c) other, being a composition of (a) and (b), or being non-price non-directive information;
- vertical and horizontal links;
- directions of control and influence.

Picking out the enterprises with the greatest differences from the average frequency of these instruments used in different directions we got four situations and kinds of enterprise behavior:

- I. The enterprise that receives from CEA more directives than any other enterprise, and is not actively in contact with CEA and other economic units. In most cases it simply implements the directives and is a subject of pressures from outside. Such firms we call "obedient".
- II. Receives as many directives as (I), but tries to exert a pressure on CEA. Most of these enterprises, called "fighting", exert also a strong pressure on other firms.

- III. The firms, that in more cases then other enterprises, receive price-type information, but are not very active in relation to CEA. Their contacts with other units are quiet, with greater role of price-type instruments. We call them "quiet".
- IV. The enterprises have rather rare contacts with CEA (in both directions), but exert a strong pressure on other firms and consumers. It is a "highly independent" enterprise.



Fixed Points, Periodic Orbits, etc., in Climatological Models

Abstract of Presentation, July 29,

J. Charney and K. Fraedrich

Following a brief review of the generation of axisymmetric circulations on a rotating sphere or in a rotating cylindrical annulus by differential heating, and their breakdown into regular and irregular waves and vortices, Lorenz' paper, "The Mechanics of Vacillation,"* was discussed as offering an example of how the topological concepts of equilibrium points, periodic orbits, etc. find their way into a model climatological problem.

Lorenz abstract is as follows (see footnote following page)**:

The equations governing a symmetrically heated rotating viscous fluid are reduced to a system of fourteen ordinary differential equations, by a succession of approximations. The equatins contain two external parameters—an imposed thermal Rossby number and a Taylor number.

Solutions where the flow is purely zonal, and solutions with superposed "steady" waves which progress without changing their shape, are obtained analytically. Additional solutions exhibiting vacillation, where the waves change shape in a regular periodic manner in addition to their progression, and solutions exhibiting irregular nonperiodic flow, are obtained by numerical integration.

For a given imposed thermal Rossby number, the flow becomes more complicated as the Taylor number increases. Exceptions occur at very high Taylor numbers, where the equations become unrealistic because of truncation.

For values of the external parameters where steadywave solutions are found, solutions with purely zonal flow also exist, but are unstable. Where vacillating solutions are found, steady-wave solutions

^{*} J. Atm. Scis., 20, 1963, 448-464.

also exist, but are unstable. A transition between unsymmetric and symmetric vacillation is not associated with the instability of either form of vacillation. It is hypothesized that where irregular nonperiodic solutions are found, vacillating solutions also exist but are unstable.

The problem of calculating unstable stationary flows and limit cycles when the boundary conditions and driving forces are not axisymmetric was then discussed.

^{**} The thermal Rossby number is a measure of the imposed horizontal temperature difference driving the relative flow in the annulus, expressed as a vertical velocity difference divided by the speed of rotation of the annulus.

The Taylor number is the reciprocal square of the logarithmic rate of frictional decay of momentum expressed in units of twice the angular velocity of the annulus.

Immunity - A Mathematical Model

A. Molchanov

(presented July 30)

I. Assumptions

Immunity may be described by two variables:

- x number of bacterias
- y number of lymphoides

Three main processes are suggested:

- A reproduction of the bacterias
- B production of the lymphoides
- C <u>destruction</u> of both the lymphoides and the bacterias as the result of the interaction.

The differential equation:

$$\frac{dx}{dt} = A - C$$

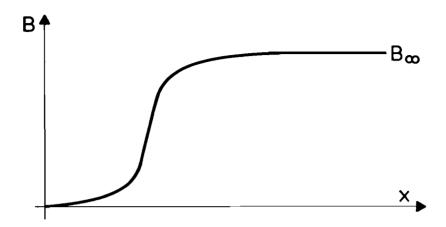
$$\frac{dy}{dt} = B - C .$$

II. A more concrete model

 $A = \alpha x$ exponential growth of the bacterias

C = yy exponential distruction of the lymphoides

B = B(x) variable level of the immunity-defense



The typical behavior of the immunity-defense depends on the number of bacterias according to the physiological principle "all or nothing."

Remarks for biologists

More realistic is a step-by-step inclusion of the various levels of immunity. The number of levels ("barriers") is large, maybe seven or more. The main properties, however, of the immunity-process in time is clear in the simple case of the one-barrier immunity.

III. Model

Variables
$$x \to \frac{x}{x_0}$$
 , $y \to \frac{y}{y_0}$, $t \to \frac{t}{t_0}$

$$\frac{dx}{dt} = \alpha x - y$$

$$\frac{dy}{dt} = \beta(x) - y .$$

Remarks for mathematicians

The system is strictly equivalent to the one describing the mechanical motion with viscosity.

Proof

$$\frac{d^2x}{dt^2} + (1 - \alpha)\frac{dx}{dt} + f(x) = 0 .$$

Here

$$f(x) = \beta(x) - \alpha x = -\frac{\partial U}{\partial x}$$

$$U = \int_{x_0}^{x} [\beta(x) - \alpha x] dx - potential function of the mechanical system$$

In the $\underline{\text{whole}}$ (x,y)-space the system has the Chetaev function (the generalization of the Ljapunov function).

Ιf

$$N = \frac{(\alpha x - y)^2}{2} + U(x) ,$$

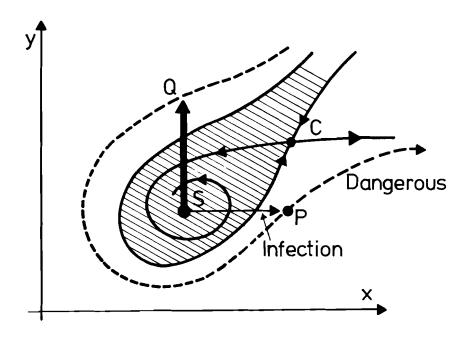
then

$$\frac{dN}{dt} \equiv (\alpha - 1)(\alpha x - y)^{2} .$$

All results about stability can be deduced from this function.

IV. Results and Phase Portraits

Weak (non-sterile) immunity

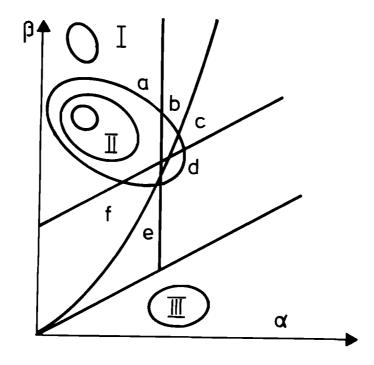


Possible result of uncontrolled use of antibiotics

- S point of non-sterile immunity (stable)
- C critical point (saddle, non-stable)
- P initial point after infection
- Q initial point after use of antibiotics

V. Results

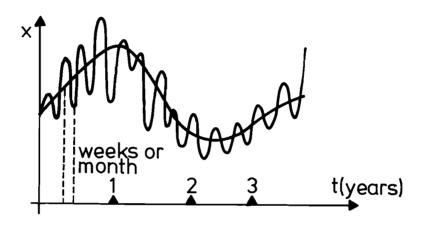
Tuberculosis immunity structures of the different populations



- I <u>Rats</u> Very strong immunity, resistence.
- III Guinea pigs No immunity.

VI. Future study

In the model presented the rapid processes are omitted. They may, however, be very important in critical situations.



The real time-dependence

The model presents the "average" description only.

A more precise model must be constructed. The process B production of the lymphoides depends essentially on the rapid variables also.

Therefore:

$$\frac{dx}{dt} = dx - y$$

$$\beta(x) = b(x,u,v)$$

$$\frac{dy}{dt} = b(x,u,v) - y$$

$$\varepsilon \frac{du}{dt} = f(s,y,u,v)$$
 ε small parameter

$$\varepsilon \frac{dv}{dt} = g(x,y,u,v)$$
 $\varepsilon \sim \frac{\text{"week"}}{\text{"year"}} \sim \frac{1}{50}$.

What are the <u>rapid</u> variables? They probably describe energy processes in the whole organism. Some biologists believe (I also) that the energy processes are connected closely with stress-events.

Time Averages Near Strange Attractors

K. Sigmund
(presented July 30)

Many dynamical systems which are structurally stable, i.e. robust with respect to perturbations of parameters, are very unstable with respect to perturbations of the initial conditions. This is particularly so in the neighborhood of strange attractors, which according to Ruelle might be relevant for the study of turbulence. "Smoothing" the system by taking long term averages seems a possible way for reducing this sensitivity with respect to initial conditions. For example, meteorologists tend to consider climate as a time average: results by Lorenz and Charney seem to point to the existence of multiple Hopf bifurcations and strange attractors for climatological models.

Let M be some "state space" and ϕ_t a one parameter group of transformations of M. The state xeM gets changed in time t into the state $\mathbf{x}_t = \phi_t \mathbf{x}$. If g is an observable (i.e. a function on M) then $\mathbf{g}(\mathbf{x})$ will be the value of the observable in the state \mathbf{x} , and $\mathbf{g}(\mathbf{x}_t)$ the corresponding value after time t. The time average is the limit of the expression

$$\frac{1}{T} \int_{0}^{T} g(x_{t}) dt , \quad T \to \infty$$

if it exists. In this case, one has a kind of statistical stability.

The principal result on time averages is the ergodic

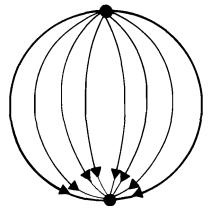
theorem: if M is a measure space ϕ_t measurable, and μ an invariant measure on M (i.e. $\mu(\phi_t A) = \mu(A)$ for all $A \subset M$ and $t \in R$) then for every L_1 function g,

$$\lim_{T\to\infty}\frac{1}{T}\int_0^T g(\phi_t x)dt$$

exists for μ almost all x.

As an example, let M be a sphere and $\boldsymbol{\varphi}_{\mathsf{t}}$ a northpole-southpole flow on M.

In this case, clearly every point has a time average.



But the ergodic theorem tells us only something about the two points N and S: indeed, any invariant measure μ must be concentrated on these two points.

We shall now describe some theorems, mainly due to Sinai, Bowen, Ruelle, which strengthen the statement of the ergodic theorem.

Thus, let M be a connected compact manifold, ϕ_t a C^2 differential flow satisfying Axiom A, and m a Lebesque measure on M (i.e. ordinary volume). Smale's spectral theorem says that the

^{*}The meaning of Axiom A is given in Walter's contribution.

nonwandering set of M can be decomposed into a finite disjoint union of invariant closed sets $\Lambda_{\hat{1}}$ which are transitive (i.e. each $\Lambda_{\hat{1}}$ is the orbit closure of some point). The $\Lambda_{\hat{1}}$ are called basic sets. One calls the sets

$$W^{S}(\Lambda_{i}) = \{x \in M : x_{+} \rightarrow \Lambda_{i} \text{ for } t \rightarrow \infty\}$$

the stable manifolds. One has

$$\bigcup_{i=1}^{m} W^{S}(\Lambda_{i}) = M .$$

The basic set $\Lambda_{\bf i}$ is called an attractor if there exists a neighborhood \cup with $\phi_{\bf t}\cup\subset\cup$ for t > 0 and $\bigcap_{{\bf t}>0}\phi_{\bf t}\cup=\Lambda.$ Ruelle and Bowen proved:

1) If Λ_i is an attractor then for m-almost all $x \in \cup$ and for every continuous observable g the time-average

$$\lim_{T\to\infty}\frac{1}{\infty}\int_{0}^{T}g(\phi_{\mathbf{t}}\mathbf{x})d\mathbf{t}$$

exists.

2)
$$M = \bigcup_{\Lambda_{i} \text{ attractor}} \overline{W^{s}(\Lambda_{i})}$$
.

- 3) If $m(\Lambda_i) > 0$ then $\Lambda_i = M$.
- 4) The basic set Λ_i is an attractor if $m(W^S(\Lambda_i)) > 0$. This satisfying picture is somewhat marred by the fact that it need not hold for C^1 flows.

If the attractor Λ_i is a fixed point y, then obviously the time-average of every point x in $W^S(\{y\})$ exists. Similarly, if

 $\Lambda_{\dot{1}}$ is an isolated periodic orbit $\gamma,$ the time-average of every point x in W^S({\gamma}) exists. But if the attractor $\Lambda_{\dot{1}}$ is not of this trivial type (if it is a "strange attractor") then the situation changes. There exist points x in the basin W^S($\Lambda_{\dot{1}}$) such that

$$\frac{1}{T} \int_0^T g(\phi_t x) dt$$

does not converge for every continuous g. Actually these points (although of Lebesque measure 0) are dense in $\Lambda_{\bf i}$. It follows in particular that an arbitrarily small change of the initial state of the system might change drastically the behavior of the time-average. One can say that one has no "Ljapunov stability in the mean".

Similar instability results hold for the time evolution of statistical states. The reason for this unstable behavior of time-averages lies in the fact that $\Lambda_{\hat{\mathbf{1}}}$ supports a very large number of invariant measures. There are infinitely many periodic orbits filling $\Lambda_{\hat{\mathbf{1}}}$ densely.

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IIASA GENERAL SEMINAR, SCHLOSS, JULY 28

On Stochastic Stability and Resilience

Yu. Rozanov

Stochastic Stability

Stochastic stability concerns a dynamic system \dot{x} = f(t,x) under a stochastic disturbance " δ ":

$$\dot{x} = f(t,x) \rightarrow \dot{x}^{\delta} = f^{\delta}(t,x^{\delta})$$
.

In addition to deterministic Stability Theory it involves many important aspects and fundamental results of

- *Markov Processes Theory (diffusion, ergodic properties, etc.)
- *Asymptotic Theory of Partial Differential Equations

Example:
$$\frac{d}{dt} = f(x)\frac{d}{dx} + \varepsilon \frac{d^2}{dx}$$
, $\varepsilon \rightarrow 0$

- *Spectral Theory of Stationary Randon Processes
- *General Ergodic Theory

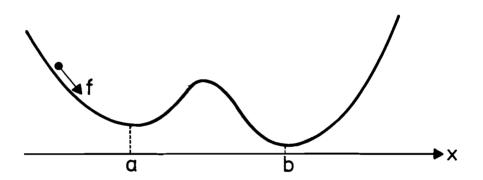
1. Typical Phenomena

Let us consider a system

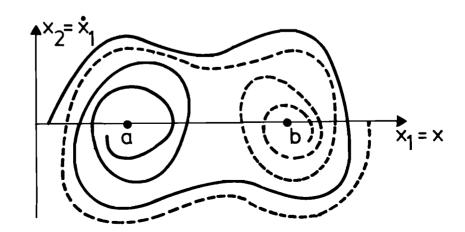
$$\dot{x} = -2k\dot{x} + f(x)$$

with a "potential"

$$V(x) = \int_{x_0}^{x} f(\xi) d\xi$$
 (see figure)



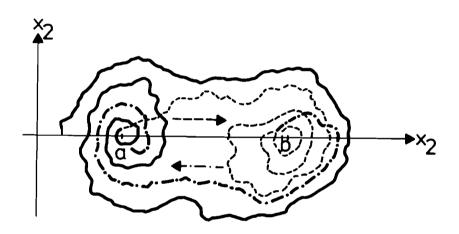
It has two equilibrium states "a" and "b".



A stochastic system

$$\ddot{x} = -2k\dot{x} + f(x) + \delta \dot{W}$$

(with a random disturbance term $\delta \hat{W})$ may behave as shown in the following figure:



Here "a" and "b" are pseudo-equilibrium states.

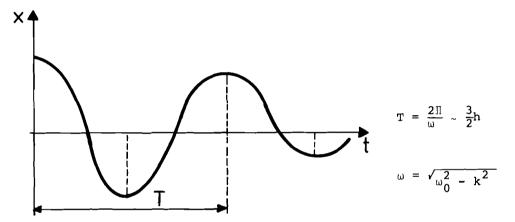
2. "White Noise" Approach

Example: Let us consider a pendulum on a ship (Gyrocompass) described by the system

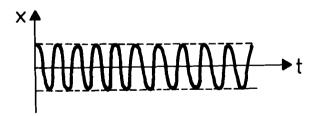
$$\dot{\mathbf{x}} + 2\mathbf{k}\dot{\mathbf{x}} + \omega_0^2 \mathbf{x} = \delta \dot{\mathbf{W}}$$

where $\delta \hat{W}$ means "sea disturbance."

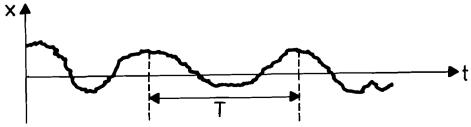
The first figure shows free oscillation:



The second one shows forced oscillation with a high frequence Ω >> ω of sea waves:



But a real trajectory looks as if the system is disturbed by "white noise" $\delta \dot{\tilde{W}}.$



3. Stochastic Linear Systems

Suppose we deal with a system

$$\dot{x} = Ax$$
 , $x \in \mathbb{R}^n$,

which has a global equilibrium $x_t^* = 0$ (all A-eigenvalues are negative):

$$x_t(x_0) - x_t^* \rightarrow 0$$
 , $t \rightarrow \infty$

$$\forall x_0 \in R^n$$
.

Let us consider a stochastic system

$$\dot{x} = Ax + \delta \dot{W}$$

where

w = standard "white noise"

 δ = a constant n x n - matrix.

Then there is a stationary (random) process x_t^* such that

$$x_t(x_0) - x_t^* \rightarrow 0$$
 , $t \rightarrow \infty$

for the system trajectory $\mathbf{x_t}(\mathbf{x_0})$ with an initial state $\mathbf{x_0} \ \epsilon \ \mathbf{R}^n$.

Here $\mathbf{x}_{\mathsf{t}}^*$ can be interpreted as a <u>statistical equilibrium</u> and it is distributed as the Gaussian stationary process with a spectral density

$$f_{\lambda} = \delta[(i\lambda E - A)(i\lambda E - A)*]^{-1}$$

and the correlation function

$$\dot{B}_t = AB_t$$
 , $t \ge 0$.

(E denotes the n x n unit matrix.)

4. Statistical Equilibria and Invariant Distributions

The system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \delta(\mathbf{x})\dot{\mathbf{W}}$$
, $\mathbf{x} \in \mathbf{M}$

determines \mathbf{x}_{t} as a Markov diffusion process on the manifold M ϵ R. Let us set

$$P_t(\Gamma, x_0) = P\{x_t \in \Gamma \mid x_0\} = \int_{\Gamma} p(x_0, t, x) dx$$
.

The transition density $p(\cdot,t,x)$ satisfies the Kolmogorov-Fokker-Planck equation

$$\frac{dp}{dt} = -\sum_{i} \frac{d}{dx_{i}} (f_{i}p) + \sum_{i,j} \frac{d^{2}}{dx_{i}dx_{j}} (b_{ij}p)$$

where

$$||\mathbf{b}_{ij}|| = \delta(\mathbf{x}) \cdot \delta(\mathbf{x})^*$$

is a diffusion matrix. Under certain conditions, $\frac{dp}{dt} = 0$ gives us a stationary solution p = p* or a statistical equilibrium p* such that

$$P_t(\cdot,x_0) \rightarrow P^*(\cdot)$$
 , $t \rightarrow \infty$

5. Asymptotical Behavior of Invariant Distribution P*

Let us consider the system

$$\dot{\mathbf{x}} = \mathbf{f}(\mathbf{x}) + \delta \dot{\mathbf{W}}$$
, $\delta = \text{const.} \rightarrow 0$

and its invariant measure $P^* = P^*_{\Lambda}$ in the case of a potential field

P* asymptotically concentrates near the set

$$\Gamma^* = \{x^* : V(x^*) = \min_{x} V(x)\}$$

namely

$$\int\limits_{R^n-\Gamma_-} p^*(\mathbf{x}) d\mathbf{x} \to 0 \quad , \qquad \delta \to 0$$

$$V\Gamma \supset \Gamma^*$$
 , Γ = open set

Note:
$$||b_{ij}|| = E$$
, $p*(x) = C \exp \left\{-\frac{2V(x)}{\delta^2}\right\}$.

6. "Pre"-asymptotical Behavior

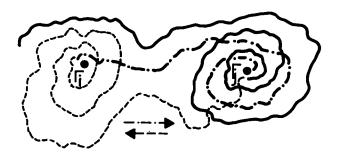
Let

$$\dot{x} = f(x)$$
 , $x \in M$

be a deterministic system with a compact phase space M and Γ_1,\ldots,Γ_m be a finite number of its ω -limit sets.

Let us consider a corresponding stochastic system

$$\dot{x} = f(x) + \delta \dot{w}$$
, $\delta \rightarrow 0$.



As shown on the picture the limit sets Γ_i , Γ_j look like <u>pseudo-equilibria</u>.

It might be shown that "jump" probabilities asymptotically are

$$P(\Gamma_i \rightarrow \Gamma_j) \sim \exp \{-v_{ij} | \delta^2\}$$

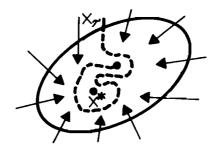
where

$$V_{ij} = V(x_{i}, x_{j}); x_{i} \in \Gamma_{i}, x_{j} \in \Gamma_{j}$$

and the function V(x,y) is determined by the system $\dot{x} = f(x)$. (Ventzel, Freidlin (1969))

7. Diffusion Against the Deterministic Flow

Let us consider a deterministic <u>inflow</u> $\dot{x} = f(x)$ in a region G with a single attractor x^* (all trajectories go into G!).



The corresponding stochastic system

$$\dot{x} = f(x) + \delta \dot{W}$$

determines \mathbf{x}_{t} as a diffusion process. The important problems concern "first passage" (or "exit") time τ :

$$P_{\mathbf{x}}(\tau \leq t) = ? \qquad P_{\mathbf{x}}(\mathbf{x}_{\tau} \in \Gamma) = ?$$

$$(x = x_0)$$
 , $\Gamma \subseteq G'$ - boundary of G) .

Let us set

$$V(x) = V(0,x) .$$

Suppose there is a single min point

$$y*: V(y*) = \min_{y \in G^*} V(y)$$
.

Then for all initial states $x \in G$

$$P_{\mathbf{x}}\{|\mathbf{x}_T - \mathbf{y}^*| \ge \epsilon\} \rightarrow 0$$
 , $\delta \rightarrow 0$,

wherever $\epsilon > 0$.

Note 1. The function V(x,y) is defined as

$$V(x,y) = \inf_{\phi} \int_{0}^{T} ||\dot{\phi}_{t} - f(\phi_{t})||^{2} dt$$

where

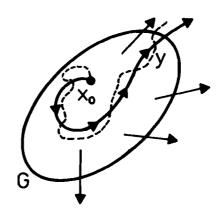
$$\phi_0 = \mathbf{x}$$
 , $\phi_T = \mathbf{y}$, $0 \le T < \infty$.

Note 2. Diffusion along the deterministic flow is a trivial case. Let

$$y* = x_t(x) \in G'$$

be the deterministic "exit". Then

$$P_{\mathbf{x}}(|\mathbf{x}_{T} - \mathbf{y}^*| \ge \varepsilon) \rightarrow 0$$
 , $\delta \rightarrow 0$.



This is obvious!

8. Structural Disturbance of a Linear System

$$\dot{x} = Ax$$
 , $x \in R^n$.

Suppose

$$A \rightarrow A + \delta \dot{W}$$

where $\mathring{\textbf{w}}$ is a standard m-dim. "white noise", so the system considered is

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \delta \mathbf{x} \dot{\mathbf{W}} \quad ,$$

δx ix an n x m matrix with elements

$$(\delta x)_{ik} = \sum_{j=1}^{n} \delta_{ik}^{j} x_{j}$$
.

Then x_t is a Markov diffusion process with <u>absorbing state</u> $x^* = 0$. Let us set

$$\rho_t = \log |x_t|$$
 , $\lambda_t = \frac{x_t}{|x_t|}$.

<u>Suppose</u> the diffusion matrix $B(x) = (\delta x)(\delta x)^*$ is non-degenerate in the sense that

$$(B(\mathbf{x})\lambda,\lambda) \geq b|\mathbf{x}|^2|\lambda|^2$$
, $b > 0$.

Then λ_{t} is a Markov ergodic process on the sphere S with invariant distribution P*.

Stability and Non-Stability

Let us set

$$I = \int_{S} Q(\lambda) P^*(d\lambda)$$

where

$$Q(\lambda) = (A\lambda, \lambda) + \frac{1}{2}TrB(\lambda) - (B(\lambda)\lambda, \lambda) .$$

Then

I < 0 → Stability:</pre>

$$x_t \rightarrow x^* = 0$$
 , $t \rightarrow \infty$

I > 0 → Non-Stability:

$$x_t \rightarrow \infty$$
 , $t \rightarrow \infty$, $(\forall x_0 \neq 0)$

I = 0
$$\rightarrow \rho_t$$
 = log $|x_t|$ - recurrent diffusion process

$$-\infty$$
 < ρ_{t} < ∞ , with repelling boundaries "- $\!\omega$ ", "+ $\!\omega$ "

(Khasminsky (1960-1967))

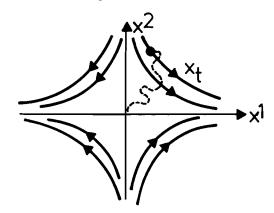
9. Stochastic Stabilization

Example

Let us consider a deterministic system

$$\dot{x}^1 = a_1 x^1$$
, $\dot{x}^2 = -a_2 x_2$, $(a_1, a_2 > 0)$

with $x^* = 0$ as a saddle point



Let us consider a stochastic system

$$\dot{x}^1 = a_1 x^1 + \delta x \dot{w}$$
, $\dot{x}^2 = -a_2 x^2$

such that

$$a_1 < \frac{\delta^2}{2} .$$

Then $x_t^1(x_0^1 > 0)$ is a diffusion process with <u>repelling</u> boundary "+\omega" and <u>attracting</u> but non-attainable boundary $x^* = 0$, i.e., with probability $1 \times_t \to 0$ but the trajectory never hits the point $x^* = 0$, $\forall x_0$. (See, for example, Prokhorov, Rozanov, "Random Processes", Springer-Verlag, 1969.)

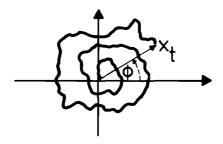
10. Stochastic Spirals

Let

$$\dot{\mathbf{x}} = \mathbf{A}\mathbf{x} + \delta \mathbf{x} \dot{\mathbf{W}}$$

be a stable planar system and

$$\varphi_{\text{t}} = \varphi + 2k_{\text{t}}\pi$$
 , k_{t} - algebraic sum of ± rotation \vec{x}_{t} (see figure).



Then

$$\dot{\phi} = a(\phi) + b(\phi)\dot{W}$$

is a diffusion process.

Suppose

$$B(x) = (\delta x)(\delta x) * is non-singular$$
.

Let us set

$$\Lambda = \int_{0}^{2\pi} \frac{a(\phi)}{b(\phi)} d\phi \quad .$$

The following statements hold true:

$$\Lambda > 0 \rightarrow \begin{cases} "-\infty" - \text{repelling bound} \\ "+\infty" - \text{attracting bound} \end{cases}$$

$$\Lambda < 0 \Rightarrow \begin{cases} "-\infty" - \text{attracting bound} \\ "+\infty" - \text{repelling bound} \end{cases}$$

$$\lim_{t\to\infty}\frac{\phi_t}{t} = (\text{sign }\Lambda)\frac{2.\pi}{E\tau}$$

where

$$\tau$$
 = "rotation time", i.e., $\phi_{\tau} = \phi_0 \pm 2\pi$

(Khasminsky, (1969)

Freedman, Pinsky, (1974)).

11. Stochastic Lyapunov Function

Let x_t be a general Markov process and A - its infinitesimal operator. Examples:

1)
$$\dot{x} = f(x)$$
, $A = \sum_{i} f_{i} \frac{d}{dx_{i}}$

2)
$$\dot{x} = f(x) + \delta \dot{w}$$
, $A = \sum_{i} f_{i} \frac{d}{dx_{i}} + \sum_{i,j} b_{ij} \frac{d^{2}}{dx_{i}dx_{j}}$

Definition of Lyapunov function:

$$V(x) \ge 0$$
 , $v(0) = 0$

$$AV(x) \leq 0$$
 , $x \neq 0$.

It is a positive superharmonic function.

Stochastic Stability

The following result holds true:

$$P_{\mathbf{x}} \{ \sup_{t \ge 0} V(\mathbf{x}_{t}) > \epsilon \} \le \frac{V(\mathbf{x})}{\epsilon}$$
 (x = initial state).

For arbitrary small probability p ther is a neighborhood $U(p,\epsilon)$ of $x^*=0$ such that $V(x)\leq p$ ϵ , x ϵ U. Thus if x ϵ U then almost for sure x_+ , $t\geq 0$, does not leave $G_{\epsilon}=\{y: V(y)<\epsilon\}$.

Stochastic Asymptotical Stability

Let V be a Lyapunov function. Then $V(\mathbf{x}_{\mathsf{t}})$, $\mathsf{t} \geq \mathsf{0}$, is a supermartingale, and

$$P_{\mathbf{x}} \{ \sup_{t \geq T} V(\mathbf{x}_t) \geq \varepsilon \} \leq \frac{E_{\mathbf{x}} V(\mathbf{x}_T)}{\varepsilon}$$
.

(E $_{\mathbf{x}}$ denotes expectation value over all x.)

One can verify that

$$\phi_t = T_t V(x) \stackrel{\text{def}}{=} E_x V(x_t)$$
 , $t \ge 0$

$$\frac{d}{dt}T_tV(x) = AT_tV(x) = T_tAV(x) ,$$

and if

$$AV(x) \leq -kV(x)$$

then

$$\dot{\varphi}_{\text{t}} \, \stackrel{<}{\scriptstyle -} \, k \varphi_{\text{t}}$$
 , $\varphi_{\text{t}} \, \stackrel{<}{\scriptstyle -} \, C e^{-kt}$.

(Khasminsky (1960-1969)

Busy (1965)

Kushner (1967)

and others.)

IIASA SEMINAR, WATER PROJECT, SCHLOSS, JULY 31

Elementary Model of Eutrophication

A. Bazykin

The pollution of water by biogenic compounds leads first to enrichment of the water ecosystem, but when the concentration of biogenic elements exceeds a threshold value the ecosystem breaks down. Frequently the rise and fall in density of some species is observed before degredation of the ecosystem.

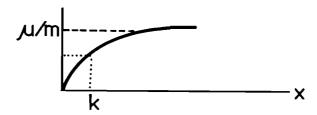
The simple mathematical model which <u>qualitatively</u> describes and in some sense explains those phenomena is presented.

Let us consider a body of flowing water with complete mixing which is occupied by an ecosystem including only two trophical levels: phytoplankton and zooplankton. The phytoplankton consume biogenic elements, the zooplankton eat phytoplankton.

Suggestions

Let us suppose:

1. The consumption of biogenic elements by phytoplankton, and of the phytoplankton by zooplankton is described by the kind of curve shown graphically.



The special analytical form is not important (and it is not known anyhow). For instance it may be dependence of Michaelis-Menten's type.

2. The coefficient of matter transformation from level to level is constant.

Then the ecosystems's dynamic is described by the following system of differential equations:

$$\dot{s} = D(s_0 - s) - \mu_1/m_1 \frac{sx}{k_1 + s}$$

$$\dot{x} = \frac{sx}{k_1 + x} - \mu_2/m_2 \frac{xy}{k_2 + x} - Dx$$

$$\dot{y} = \mu_2 \frac{xy}{k_2 + y} - D_y$$

where s, x, y denote concentrations of biogenic elements, phyto- and zooplankton, respectively.

D - the velocity of flow

s - initial biogenic concentration

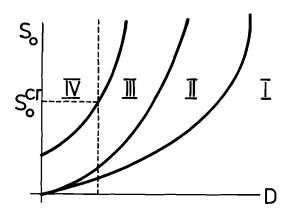
 $\boldsymbol{\mu}_{1}\text{, }\boldsymbol{\mu}_{2}\text{ - maximal rates of reproduction}$

 m_1 , m_2 - coefficients of the transformations: biogenic to phyto- and phyto- to zooplankton

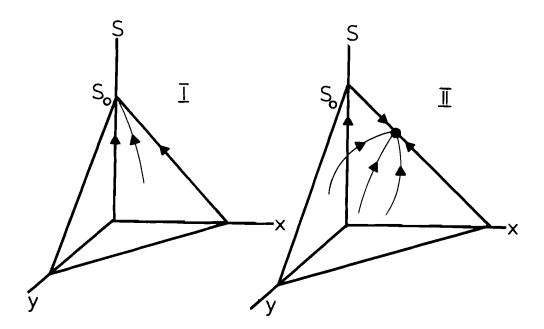
 k_1 , k_2 - Michaelis constants, describing saturation effects.

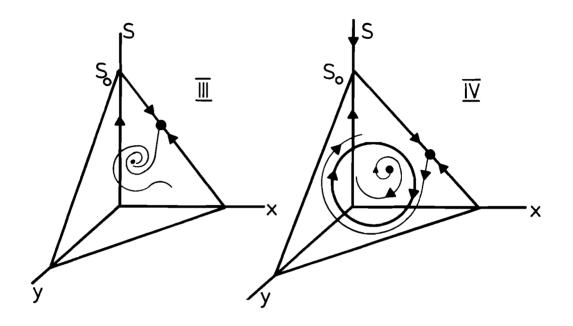
We have an eight-dimensional parameter space and a threedimensional phase space. Unfortunately, it is the simplest of possible descriptions of the situation. Changing the scale of s, \mathbf{x} , \mathbf{y} and \mathbf{t} we can reduce the number of parameters to four.

The structure of the parameter space is described completely by the two-dimensional projection to the plane (D,s $_{
m O}$).

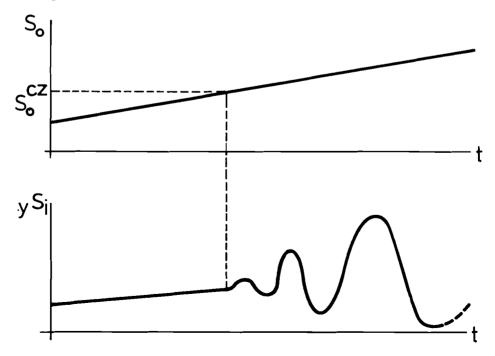


The phase behavior in regions I-IV are the following:





Let us slowly increase \mathbf{S}_0 , then the behavior of zoo- (and phyto-) plankton density will be the following:



Conclusion

The presented model explains some main properties of man-made eutrophication.

IIASA GENERAL SEMINAR, SCHLOSS, JULY 31

Jule G. Charney

Drought as a Biogeophysical Feedback Mechanism

Changes in surface albedo cause an immediate change in energy received from the sun and therefore, if widespread, can have a potentially very great influence. It may be expected that regional albedo changes will have an appreciable effect on regional circulations. In the Royal Meteorological Society's Symons Memorial Lecture for 1974 Charney (2) discussed a biogeophysical feedback mechanism which tends to produce changes in rainfall and plant cover. This mechanism operates because of the dependence of the surface albedo on plant cover. covered by plants has an albedo in the range of 10 to 25 percent, whereas ground with no vegetation frequently has a higher albedo, as high as 35 to 40 percent in the case of dry, light, sandy Thus a decrease in plant cover may be accompanied by an increase in the surface albedo. This would lead to a decrease in the net incoming radiation and an increase in the radiative cooling of air. As a consequence, the air would sink to maintain thermal equilibrium by adiabatic compression, and cumulus convection and its associated rainfall would be sup-The lower rainfall would in turn have an adverse effect on plants and tend to enhance the original decrease in This positive feedback will be particularly important in regions such as the Sahara where (i) large-scale subsidence already occurs; (ii) most of the rainfall is from

cumulus clouds; and (iii) transports of heat by the winds are particularly weak and inefficient at counteracting temperature changes due to albedo changes. This mechanism offers a possible explanation for past changes in the climate of the Sahara (4), and, in particular, for droughts in the Sahel (the southern region of the Sahara), where the process could be initiated or prolonged by overgrazing.

In Charney's analysis an increase in the albedo in a large region causes enhanced sinking and drying only to the extent that the temperature departs more than before from radiative-convective equilibrium, and this departure depends on the efficiency of a frictionally controlled circulation which reduces the horizontal temperature gradients that would be established by radiation alone. However, his mechanism fails to take into account the dynamical effect of the release of latent heat in precipitation and ignores the effects of the global circulation. For example, it does not take into account the interaction of the desert circulation in the Sahara with the monsoon circulation to the south.

In order to assess the plausibility of his mechanism, we need to calculate its effect together with the effect of all other mechanisms which operate simultaneously, and see if the net effect is appreciable. In the past decade computer models of the general circulation of the atmosphere have been developed which implicitly or explicitly include most atmospheric processes, winds, convection, clouds, rain, radiative absorption, and emission. In this study the general circulation model (GCM)

developed at the Goddard Institute for Space Studies (5) has been used to calculate the net effect of a change in surface albedo in the Sahel.

At the same time the albedos in two other areas, the Western Great Plains of the United States and the Thar Desert of India-Pakistan were modified. Two integrations were performed, and for both the observed state of the atmosphere for 18 June 1973 was used as the initial condition. Both integrations were carried forward for 6 weeks of simulated time. The only difference between the two integrations was the prescribed surface albedo for the Sahel, the Western Great Plains and the Thar Desert. Both integrations had boundary conditions, such as sea surface temperature and soil moisture, prescribed to correspond to climatological conditions for July (summer is the rainy season in the three areas). In one integration the surface albedo was 14 percent, and in the other it was 35 percent. simulate, repectively, a surface covered with plants and a surface devoid of plant cover. The surface albedos in the unmodified case were 35 percent over the Sahara-Arabian-Indo-Pakistani complex od deserts, the Great Western Desert of the United States and Mexico, and 14 percent elsewhere. modified case the albedos were changed from 14 percent to 35 percent in the Sahel at the southern margin of the Sahara, the Western Great Plains at the eastern margin of the Great Western Desert and in the Thar Desert at the eastern margin of the Afghanistan-Pakistan desert. The model's resolution is 4° in latitude and 50 in longitude. The actual albedo changes were

at the eleven grid points running from $15^{\circ}W$ to $35^{\circ}E$ at $18^{\circ}N$ in the Sahel, the eight grid points running from $34^{\circ}N$ to $46^{\circ}N$ at $100^{\circ}W$ and $105^{\circ}W$ in the Western Great Plains, and the four grid points, $26^{\circ}N$ $70^{\circ}E$, $26^{\circ}N$ $75^{\circ}E$, $30^{\circ}N$ $70^{\circ}E$, and $30^{\circ}N$ $75^{\circ}E$ in the Thar Desert.

The upper of Figures 1, 2 and 3 show the mean weekly precipitation averaged over the three regions from both integrations. With the exception of the second week in the Western Great Plains (here labelled, somewhat inaccurately, the "Dust Bowl"), the rainfall in the high-albedo (35 percent) experiment was substantially smaller than in the low-albedo (14 percent) experiment. With the above-mentioned exception, the consistency in the difference in rainfall suggests that the difference is real and not a result of statistical fluctuations. However, in each case the rainfall in the marginal areas was considerably higher than the observed values. This was attributed to a deficiency in the ground hydrology which gave excessive evaporation in arid regions. Accordingly, experiments were performed with essentially no evaporation from land surfaces. The results are shown in the lower half of Figures 1, 2, and 3. The latter suggest again, although not as strongly, that the rainfall reduction in the Sahel and "Dust Bowl" areas are real, but that the reduction of rainfall in the Thar Desert is questionable.

Figures 4 and 5 show the latitudinal distribution of the mean rainfall and mean vertical velocity over Africa during July in the two experiments. From $18^{\circ}N$ to $34^{\circ}N$ the values plotted are the rainfall and vertical velocity averaged over

all the grid points in the Sahara at each latitude. The shift in the rainfall distribution reflects a shift to the south of the Intertropical Convergence Zone (ITCZ) over Africa. The latitude of the mean low-level convergence over Africa during July was shifted about 4° southward by the increase in albedo in the Sahel. There was no such shift of the ITCZ over Asia in the two experiments. The high-albedo experiment appears to be the more realistic one.

It is concluded that surface albedos can have a substantial effect on climate and that the biogeophysical feedback mechanism is a plausible one for causing such changes. We can envisage overgrazing in the Sahel leading to an increase in the surface albedo which causes the ITCZ to move south and the rainfall over the Sahel to decrease, perhaps by as much as 40 percent. While there is not as much documentation for albedo changes in the "Dust Bowl" region, overgrazing and changes in land use could have contributed to drought in this area as well. Since the GCM we used does not include a model of the biosphere for calculating changes in albedo resulting from changes in rainfall, this 40 percent figure is, in effect, an upper bound on the amount that would occur if all links in the feedback mechanism were included. The need for a model of the biosphere empahsizes the complexity of climatic problems.

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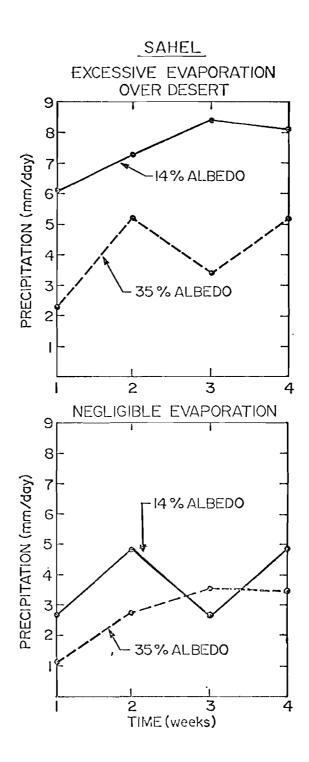


Figure 1.

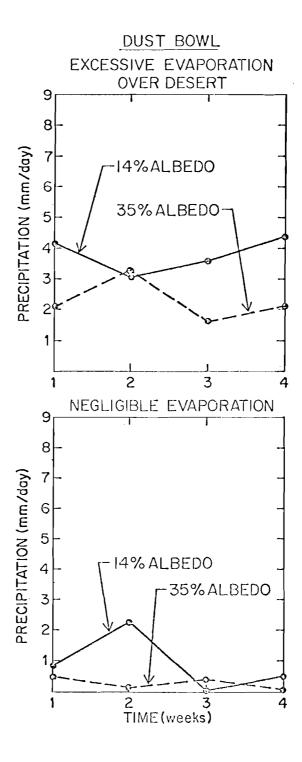


Figure 2.

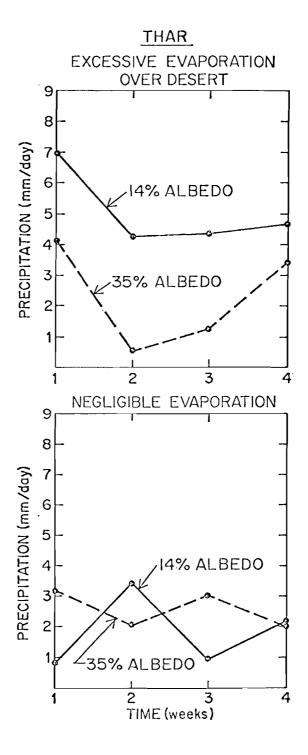
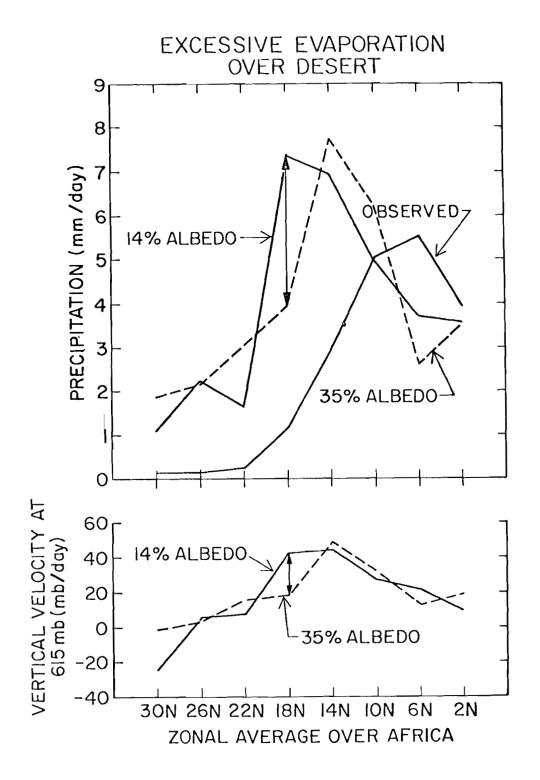
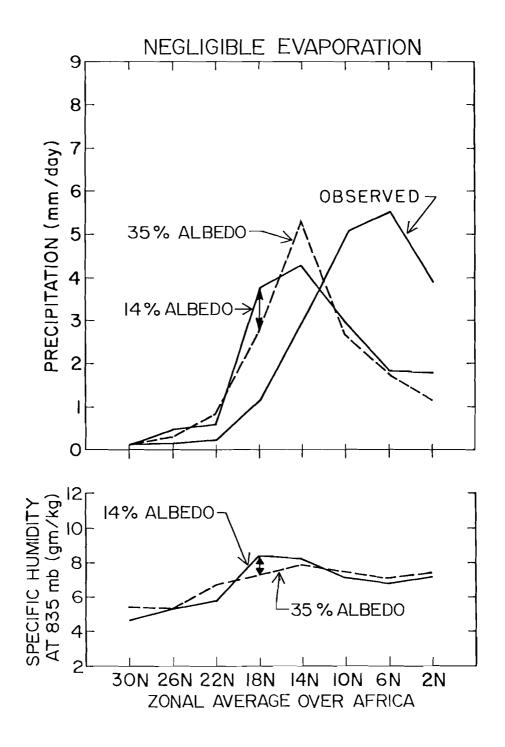


Figure 3.





MEMORANDA CIRCULATED DURING THE WORKSHOP

Rigorousness May Be Dangerous (The "Fixed-Point Ideology")

A. Molchanov

Negative Side

Consider the equation

$$\frac{d\mathbf{r}}{dt} = -\alpha(\mathbf{r}, \varepsilon) \quad . \tag{1}$$

It follows from the system,

$$\frac{dx}{dt} = \frac{\partial w}{\partial y} - \frac{1}{2x\alpha}(r, \epsilon)$$

$$\frac{dy}{dt} = \frac{\partial w}{\partial x} - \frac{1}{2y\alpha}(r, \epsilon)$$
 (2)

in the polar coordinate system,

$$r^2 = x^2 + y^2$$
 (3)

There ϵ is a small parameter (described more precisely below) and function $\alpha(r,\epsilon)$ > 0. (4)

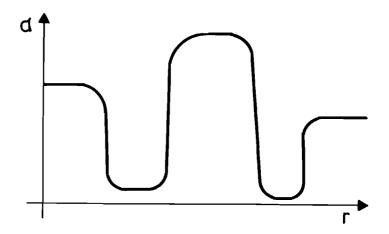
Therefore, system (2) has the Liapunov-function,

$$L(x,y) = r , (5)$$

and (1) may be regarded as the equation for the L - function of the system (2).

Hence, the system (2) has a unique fixed-point x=0, y=0 and no other fixed-points or limit cycles. All trajectories tend to this stable state of equilibrium.

Suppose, however, that $\alpha(\textbf{r},\epsilon)$ is small in some domain

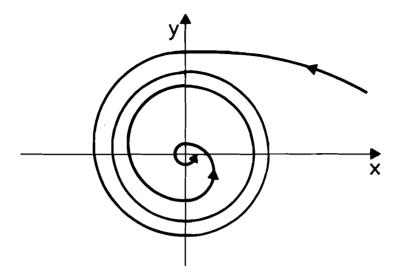


For example,

$$\epsilon \text{ if } |r-1| < \delta$$

$$\alpha(r,\epsilon) = \alpha \text{ if } |r-1| < \delta .$$

In this case, trajectories "drift" very slowly through the ring $|r\text{--}1| \; \leq \; \delta \, .$



The "through-time" T is

$$T = \int_{r_1}^{r_2} \frac{dr}{\alpha(r,\epsilon)} \approx \int_{1-\delta}^{1+\delta} \frac{dr}{\epsilon} = \frac{2\delta}{\epsilon}$$

and may be very long if ϵ is small enough.

Practically, r = 1 performs the role of a limit cycle. It is stable outside and unstable inside.

But rigorous mathematical considerations have omitted this important phenomenon.

Rigorousness May Be Dangerous But Not Necessarily

A. Molchanov

Positive Side

The construction of the previous memorandum may be generalized. Consider now any system in the n-dimension y-space,

$$\frac{d\vec{y}}{dt} = \vec{b}(\vec{y}) \quad , \tag{1}$$

and construct a new system

$$\frac{d\vec{x}}{dt} = \vec{a}(\vec{x}) \tag{2}$$

by multiplying with the positive scalar function α ,

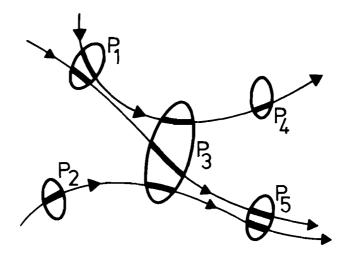
$$\alpha(\mathbf{x}) > 0$$
 (3)

so that

$$\overset{\rightarrow}{\alpha}(\overset{\rightarrow}{\mathbf{x}}) = \alpha(\overset{\rightarrow}{\mathbf{x}})\overset{\rightarrow}{\mathbf{p}}(\overset{\rightarrow}{\mathbf{x}}) \quad , \tag{4}$$

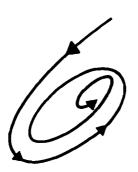
System (2) has the same trajectories as (1), but the velocity depends on the value $\alpha .$

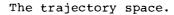
Suppose, as in N, α is small in some domains

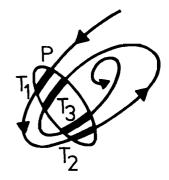


 P_i - domains, where α is small and, hence, "through-drift" is slower.

Such domains are similar to the quasi-particles in physics



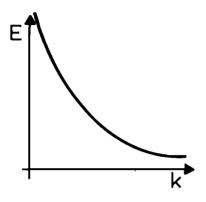


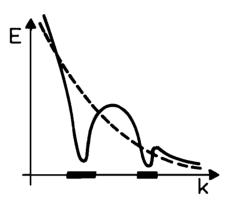


The same trajectory in x-space. The quasi-particle P has an infra-structure. Its "life-time T \approx T₁ + T₂ + T₃.

Unhomogeneous Turbulence (Hypothesis)

The developed approach may be helpful to the problem of the relation between homogeneous and unhomogeneous turbulence.





The energy-flow in the theory of homogeneous turbulence.

The possible influence of the boundary conditions.

The domains in k-space, where the energy-flow is small, may correspond to the metastable macromotions, such as curls of ellipsoidal motion (in the sense of A.M. Obuchov). I believe that this approach is very close to the one of Obuchov.

The quasi-particles in this case are very complicated motions in the three-dimensional domains with relative weak interaction.

The theory of non-linear oscillations is probably applicable to such problems.

If the developed picture corresponds in anyway to the "reality" this approach must be helpful in other problems, in particular, ecological ones.

Stability versus Resilience

A. Molchanov

Abstract

The complexity of biological systems (their structural hierarchy) points out dynamically the time-scales hierarchy of different processes.

This leads to the hierarchy in the motion of stability.

Rapid processes do not have full y stable, but "metastable" states and evolve slowly into the exact equilibrium state.

The notion "lability" (well known in medicine) reflects the existence of the surface of the possible quasi-equilibrium states.

Resilience (in my opinion) is only a particular case (and not defined rigorously) of the notion "adaptivity" (also well known). But the definition of adaptation follows from the idea of stability, which is presented more precisely below.

Hierarchy of Time Scales

I. Rapid and Slow Variables

Correct models of biological (ecological, in particular) systems usually contain a small parameter $\boldsymbol{\epsilon}$

$$\frac{d\vec{x}}{dt} = \varepsilon \vec{a} (\vec{x}, \vec{y})$$

$$\frac{d\vec{y}}{dt} = f(\vec{x}, \vec{y}) + \varepsilon \vec{b}(\vec{x}, \vec{y})$$
 (1)

where ϵ is the ratio of characteristic times

$$\varepsilon = \frac{"y - time"}{"x - time"} . \tag{2}$$

Rigorous study of such systems was begun in the well-known work of A.N. Tikhonov. The trajectories structure can be found supposing that ϵ = 0

$$\frac{d\vec{x}}{dt} = 0$$

$$\frac{d\vec{y}}{dt} = f(\vec{x}, \vec{y}) . \tag{3}$$

In the new system vector \vec{x} is constant,

$$\vec{x} = constant = \vec{\alpha}$$
 (4)

and, consequently, performs the role of a parameter

$$\frac{d\vec{y}}{dt} = f(\vec{\alpha}, y) . \tag{5}$$

Stationary state of this system are found from the equation

$$f(\vec{\alpha}, \vec{y}) = 0$$
.

Let us consider the simplest possiblity when \vec{y} and $\vec{\alpha}$ are scalars. Even in this case, the set of stationary states is not a discrete collection of isolated fixed-points but a continuous curve on the surface (α,y) .

Just the rich structure of equilibrium (to be more exact, quasi-equilibrium) state sets determines the complexity of the stability area concept.

For instance, let the equation $f(\alpha,y)=0$ have a number of solutions with different α ,

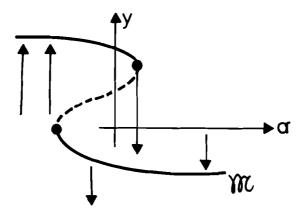


Figure 1.

Two semi-infinite branches of stable quasi-equilibria are connected by the arc of unstable ones. The upper branch corresponds to the "working-state" of the system, the lower branch describes the possibility of hysteresis.

II. The Evolution System

Now remember that the system (5) approximately describes a complete system. We shall bring back a slow <u>evolutional</u> motion. In our simplest case it is enough to solve a quasiequilibrium equation

$$f(x,y) = 0 , (7)$$

$$y = \gamma(x)$$

and to introduce y into the first equation of the exact system

$$\frac{dx}{dt} = \varepsilon \alpha(x, \gamma(x)) .$$

One should keep in mind that evolution takes place in a different way on each of the branches of the quasi-equilibrium curve

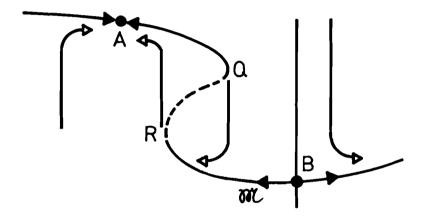


Figure 2.

with approximate equilibrium on the curve M of metastable states. On the upper brance the exact state (A) is stable, on the lower one it is unstable (B).

III. External Perturbations

Let us analyze the situation depicted on Figure 2 in a more detailed manner and show that knowing the curve M and the points A, B, Q on it fully determines the system behavior with regard to perturbations.

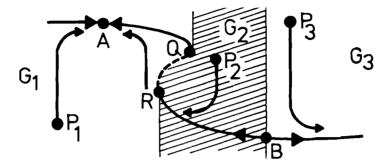


Figure 3. Splitting of the curve M into three branches: AQ_1 is a metastable brance, RB an adaptive brance and BB an unstable branch.

If the perturbation moves the system to any point of G_1 area then its future will be the same as for the point P_1 .

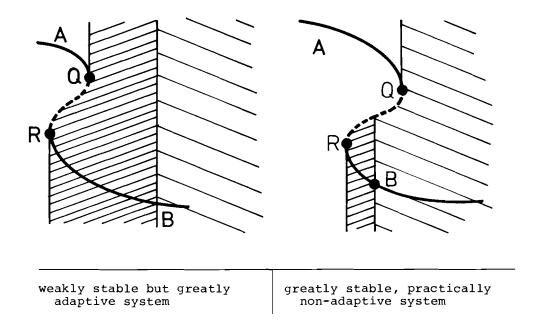
The system will rapidly move to the upper "work-branch" of the curve M and will slowly return to the exact state of equilibrium.

Point P_2 is a typical representative of the G_2 area. The events take a different turn. The system rapidly falls into the "shock-state", remains in it for a long time (while the evolution $R_2 \rightarrow R$ is taking place), but in the long run, "collects its strength" and returns to the "work branch" and only to the point S. Then slow restoration takes place, that is evolution $S \rightarrow A$.

Coming to \mathbf{G}_3 area means death of the system if we mean by this the impossiblity to return to the work state that is on the upper branch.

IV. Stability and Adaptivity

Mutual disposition of the points A and B on the curve M can greatly change the character of the system reaction to perturbation.



Comparing these two figures reveals an important difference between adaptive and stable figures.

The adaptive system "falls into a shock state" already in case of small perturbations but is able "to recover" even after strong shocks.

The stable system without adaptation on the contrary, preserves its "working ability" even in case of great perturbations but falling into a shock state almost means death for it.

V. Resumé

The concept of resilience is related to the concept of metastability of a rapid motion rather than to the traditional concept of stability. The contrasting of resilience and stability arises

if slowly changing variables are treated as parameters but everything implicitly takes its own place if evolutionary system variations are taken into consideration.

A general stability concept may reasonably be specialized for systems with a time-scale hierarchy. The concept of meta-stability may be reserved for describing stability of cut down systems of rapid motions.

A stability of slow motions may be described by the well-known term "adaptivity."

The term "resilience" may be used as a synonym of adaptivity for the particular case of ecological systems.

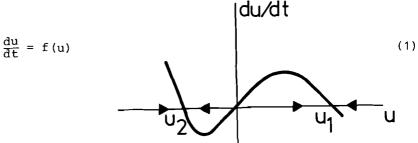
Such an approach allows for a rigorous definition of the resilience concept which previously was introduced at an intuitive level.

Equilibria in Local and Distributed Systems

A.D. Bazykin

Dr. C. Walters in his lecture of July 21 and Prof. P. Schuster in his remarks after Dr. H. Grümm's lecture of July 23 attached attention to the importance of studying not only local equilibria but also equilibria (and cyclic phenomena) in systems with distributed variables. I formulate a question from an ecologist to a mathematician.

Let us consider the simplest case:



with one-dimensional diffusion

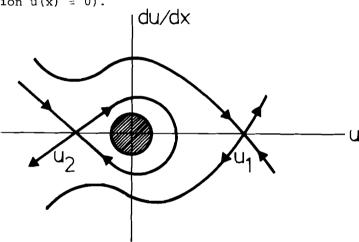
$$\frac{\partial \mathbf{u}}{\partial \mathbf{t}} = \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} + \mathbf{f}(\mathbf{u}) \quad .$$

First we are interested in the stationary solutions which are described by the equation

$$\frac{d^2u}{dx^2} = -f(u) \quad \text{or the second-order system}$$

$$\begin{cases} du/dx = p \\ dp/dx = -f(u) \end{cases}$$
 (2)

The behavior may be shown on a phase diagram, where trajectory and fixed points correspond to stationary distributions u(x) (the saddle-points correspond to stable equilibria of (1) and to stable, trivial distributions $u(x) \equiv constant$; the center corresponds to the unstable equilibria of (1) and to the unstable, trivial distribution $u(x) \equiv 0$).



As in many cases the natural boundary conditions in definite intervals are du/dx = 0, so the most interesting are $x = x_{1,2}$ the periodical solutions and the loop of separatrices.

It is possible to show by perturbation theory methods that the solution lying in the shaded area (with small amplitudes and periods) are unstable. On an arbitrary interval (if it is large enough) some stable stationary nontrivial distributions can exist.

The question to mathematicians is: how to determine the domain of attraction of each of those distributions in the infinite dimensional space of initial conditions?

It is only the first, simplest question in this field. The more interesting (and complex) problems arise if we consider:

- running waves (very interesting for application)
- 2. two-dimensional diffusion
- 3. more than one dynamic variable.

CLOSING PLENARY SESSION, SCHLOSS, JULY 31, AM

What Have We Learned?

Tjalling C. Koopmans

Koopmans: The workshop, I recall, started from the observation that there seemed to be mathematical and computational problems common to a number of different subject matter fields. We therefore hoped that there might be a benefit in bringing together people who do modelling in various areas and people who work on alternative algorithmic approaches and on the mathematical conceptualizations needed in connection with these equilibrium and dynamic models. In my perception of the experiences in the workshop, we have had good luck and this has turned out to be the case. There were a number of parallels between the different fields of application. The analogies that came out most clearly in the workshop are those between climatology and ecology. also found that the concepts of purely mathematical fields, such as differential topology, and the various ways of describing dynamic systems with continuous time and with discrete time, deterministic and stochastic, actually form a strong bond between the several fields of application. Our main problem was how to divide the time between sessions where we talked to each other and time where individuals worked by themselves, or in groups of two or three.

I said already that the applications considered were mostly climate and ecology, with some discussion of problems of chemical evolution as well. We also had economists represented.

A majority of those doubled as algorithmists or organizers, and

were in demand on that score to such an extent that they had little time for work specifically in economics. The only economist functioning as an economist in our midst was Professor Beksiak from Poland, who contributed from his experience with empirical problems of economics that bear on the estimation of equilibria.

We cannot, of course, expect to show "results" from two weeks of interaction. We do feel that we gained information about each others fields and methods, we gained insight about our common problems. We also arrived at some conjectures about how to adapt or extend algorithmic procedures to the unsolved problems that came to the fore.

I call first on Professor Charney.

Charney: To answer the question of what we have learned I would like to say for myself that I found the workshop exceedingly stimulating and that it greatly broadened my view of the problems of geophysical fluid dynamics, especially of turbulence. I agree with Prof. Koopmans that to find other groups with very different models talking about the same kind of mathematical problem is extremely useful for one's perception of one's own field. I would like to congratulate him for keeping the workshop on a constructive course when, because of so many different points of view, it could easily have become a tower of Babel.

I have come away with the feeling that the concepts of differential topology should and will become more and more important in dynamical meteorology and oceanography. The point of view which I think we should take in approaching the problem

of the dynamical modelling of climate was well exemplified by Dr. Grümms review of the paper by Ruelle and Takens "On the nature of turbulence." When the limit cycles themselves become unstable and give rise to something called turbulence, the points in the phase space still cluster around the unstable limit cycle. The orbits are no longer periodic but remain localized on a subset in the phase space. I find this concept, though still vague to me, to fit very well my own intuitive thinking about how to avoid having to play very expensive and time-consuming Monte Carlo games with general circulation models, especially when one is not even sure that one is dealing with a transitive* system, or even with one that has a statistically stable limit. There must be an alternative approach, and the one that looks most promising is to calculate first the fixed points beyond the limit where they become unstable, then calculate limit cycles by perturbation methods and finally to extend the calculations beyond the point where these, too, become unstable. My hope is that they will somehow remain central to the phase-space torus on which the actual motion takes place. If we can do this, we will have achieved a great deal more in developing a theory of climatology than anything that has been done in the past. The problem looks feasible though difficult.

Many of the ideas which were mentioned in other contexts, e.g., Dr. Rozanov's discussion of stochastic processes which convert intransitive into transitive systems, seem to me important.

^{*}The term "transitive", introduced by Prof. Lorenz, refers to a dynamical system which is governed by equations whose solutions may be extended indefinitely into the future and have statistical properties which are independent of the initial conditions.

Let me finally refer to the discussion of computational methods by Scarf, Hansen, Grümm and others. The methods that were discussed seem most applicable when one has a fairly small number of degrees of freedom. But they may also be appropriate to the meteorological problem because it is often possible to simplify the problem by introducing functional representations which reduce the dimensionality of the phase space. Other methods, such as the backwards-forwards false time extrapolation of Rivas are local rather than global in character and may require first a global calculation such as Scarf's to localize the approximate positions of the limit points and cycles.

Fraedrich: I do not need to repeat that what Dr. Charney said and only want to add a few aspects of application of fixed points methods to climatological problems, e.g., a problem that has been turned out by Prof. Charney's lecture this morning, the problem of looking for feedback systems in regional climatology as has been mentioned also in some work in the Institute and also some work on Blake's "The Feedback of Meteorological Dynamical Systems with Hydrological Systems" and may possibly be extended to ecological systems, that is, to a further field of application, to regions where there is data available to verify the findings experimentally. A second aspect which I want to mention as it fits in with the paper that has been introduced to me for the first time by Dr. Grümm seems to be the conviction that the fixed point methods and the mathematical factors of different set stages of structure can

be applied to these hydrodynamic systems which are caused by buoyancy. I think these two aspects are thought to be in addition to that which Dr. Charney said and may be looked into further.

Koopmans: Thank you very much. We have some time for discussion.

Anyone who would like to raise a question or make a comment?

Charney: From the general mathematical point of view, I am

intrigued by the role of symmetry. In the problem that Prof. Fraedrich mentioned, convection between parallel planes, the

breakdown of stability appears as an infinity of steady circulations, e.g., in some phase space as a set of fixed points

which, however, lie in a continuous line. But this property depends very strongly on symmetry. Without symmetry it is a question as to whether more than one stable fixed point exists. The same problem occurs in the Lorenz model. Here you have translational symmetry, and the first breakdown of stationary flow appears as a steady translating wave. I think, since the real climatological problem lacks these symmetries, that this special case would be bypassed, e.g., the breakdown of stability would appear first as a limit cycle rather than as a fixed point in a translating coordinate system. The problems of transitivity are also related to the various symmetries and I think are worth mathematical investigation.

Grdmm: I think there is some information on these problems of spontaneous breakdown of symmetry from theoretic physics, although in a different connection. Maybe the concepts from this field could be taken over to this question. But on the other hand

these problems won't lead very easily to computation because a continuous symmetry breaks down and you will certainly have a one-parameter family of fixed points or closed orbits.

<u>Koopmans</u>: As there are no further questions, I now call on Dr. Penenko.

Penenko: At the very beginning I would like to make some general remarks. The main attention of our workshop was devoted to stability problems and interpretations of stationary solutions. But actually we dealt with the broader questions of applied mathematics. It gave us an opportunity to discuss many interesting problems. And the general point of view which we shared was the approach of applied system analysis.

Now I wish to characterize the main system approaches which were used in our group for meteorology problems at the Novosibirsk Computing Center. The first point concerns the problem itself, how to formulate a mathematical model for the real physical process description. The next step deals with discrete approximation for continuous models. And the main requirement for this discrete approximation is that the discrete model have all those features that satisfy the same physical process described in a continuous form. The most useful and successful approach was the one based on the generalized solution definition. very difficult problems connected with the discrete appoximation design were reduced to finding stationary points of some functionals. The main method for computational algorithm construction for discrete model realization is a splitting-up method. On the one hand, this method helps us to use a simple computation procedure and, on the other hand, it gives us some

new approach to a complex model design. The splitting-up method also allows us to combine different methods in one approach, for example: methods for the solution of both stationary and nonstationary problems. (It is common knowledge that the stationary solutions are connected with fixed point problems).

Let me illustrate these remarks by a few formulas: the problem

$$\frac{\partial \phi}{\partial t} + A\phi = f \qquad , \tag{1}$$

where A is any operator and f is any given vector, is nonstationary. Suppose that a stationary solution exists, and if $t \to \infty$, we will receive the solution of the stationary problem

$$A\phi = f . (2)$$

Let us write four discrete approximations which are usually used for solving problem (1)

$$\frac{\phi^{j+1} - \phi^{j}}{\Delta t} + A\phi^{j} = f \qquad 0(\Delta t) , \qquad (3)$$

$$\frac{\phi^{j+1} - \phi^{j}}{\Delta t} + A\phi^{j+1} = f \qquad 0(\Delta t) , \qquad (4)$$

$$\frac{\phi^{j+1} - \phi^{j}}{h^{t}} + A \frac{\phi^{j+1} + \phi^{j}}{2} = f \qquad 0 (\Delta t^{2}) \quad , \quad (5)$$

$$(E + t^2 B) \frac{\phi^{j+1} - \phi^j}{\Delta t} + A \frac{\phi^{j+1} + \phi^j}{2} = f \qquad 0 (\Delta t^2) .$$
 (6)

Here the symbol $0(\Delta t^k)$ k=1,2 defines the order of approximation errors. Scheme (3) is explicit, and schemes (4) to (6) are implicit. In the limit for $j \to \infty$ each of these schemes may lead to the stationary solution, and the process itself is called "the process of stationarity". Operator $(E + \Delta t^2 B)$ is called "the stabilization operator". If $\Delta t^2 ||B|| < 1$, then schemes (5) and (6) are equivalent as regards accuracy. By a special choice of the operator B, we can, on the one hand, speed up the stationary process, and, on the other hand simplify the realization of the implicit scheme (6).

Suppose, that the operator A allows a representation $A = \begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix} A_1$ where the operators A_1 ($i = \overline{1}, \overline{n}$) have a simpler structure than A. Then scheme (6) may be reduced to some splitting-up scheme, for example, the scheme of the Douglas approximation correction type,

$$\frac{\phi^{j+1/n} - \phi^{j}}{\Delta t} + \frac{1}{2}A_{1}(\phi^{j+1/n} - \phi^{j}) + A\phi^{j} = f ,$$

$$\frac{\phi^{j+i/n} - \phi^{j}}{\Delta t} + \frac{1}{2}A_{1}(\phi^{j+i/n} - \phi^{j}) = \frac{\phi^{j+i-1}}{\Delta t}(i = \overline{2}, \overline{n}) .$$

Scheme (6) and the form of operator B is obtained from (7) by elimination of functions with fractional indexes.

It is evident that scheme (7) has a simpler and more economical computer algorithm than implicit schemes (4) and (5) as, on each fractional step, a simpler problem is solved. This approach can be applied to many problems, Russian mathematicians

use this approach in meteorological, continuum mechanics, hydrodynamics problems and others.

Another short remark. The solution of stability problems is closely connected with eigenvalue problems. We developed a few numerical methods for solving eigenvalue problems which appear in meteorology. It gives us an opportunity to formulate new meteorological models of a spectral type.

General problems concerning complex systems also involve such questions as sensitivity and the range of predictability analysis connected with the insufficient knowledge of the model parameters and input data. These questions also arise in connection with problems of a spectral type. For the appropriate estimation of the effects of parameter variation it is worth while using the technique of adjoint problems of atmospheric hydrothermodynamics. The problems concerning stability related to parameter variations are closely connected with the identification model and the range of predictability. The solution of the above mentioned problems allows us to use the mathematical models for forecasting purposes.

<u>Koopmans</u>: Any questions? No, then I call on Bill Clark and Dr. Bazykin. Clark: We started out at the beginning of this workshop by telling you all that the problems we faced in analyzing ecological models were nonlinearity, discontinuity, multivariate complexity and the occasional stochastic nature of ecosystems themselves. This view, I suppose, has been more influenced by our attempts to bring fairly strict analytical techniques and later on mathematical programming to bear on some of our modeling problems, and having been knocked down repeatedly because one or more of these structural characteristics of the phenomena we tried to model. We also mentioned in passing that we were not sure if we were not concerned with slightly different behavioral properties of these models than some of the other disciplines represented here. Our focus was somewhat on stable fixed points, but as much, or more so, we were concerned with the existence and location of separatrices, periodic orbits and so forth. Now it turned out that one of the mistakes we made early on was coming into this workshop thinking we knew what we should be telling the methodology people and getting that quite back-The structural problems which had given us so much of a run-around before seem to present not overwhelming difficulties in the context of this workshop. It turned out that interest developed around the behavioral properties of the systems we were interested in analyzing. This interest provided a focus for a number of discussions as to whether one could use variants of the techniques discussed to get at periodic orbits, and whether some of the badly behaved periodic orbits that we encountered -- these due to the discrete time nature of the models--would present special difficulties.

<u>Koopmans</u>: The behavior of the individuals and of species that are in interaction?

Clark: No. The behavior of the state space.

<u>Koopmans</u>: So it is the way the vector field of the trajectories depends on the parameters of the problem that you allude to with the term "behavior?"

Clark: Yes. Now that is not a statement of what we have learned, except that we have learned of different sets of questions relevant to different people. Later on Dixon Jones and, I guess, Terje Hansen will speak briefly on some computational experience we have had, and on some leads that have been developed concerning meteorological analogies to some of these vector field behavior problems. In a more general sense it is my tentative interpretation that many of the different attitudes that we brought into the workshop come from our fundamental focus on the dynamics of the system itself as opposed to the economists focus on statics or behavior around certain fixed points. I believe we end up sharing this attitude with the climatologists. This happened in a number of other areas as well.

We have found a great number of apparent similarities between the climatological fluid dynamics problems and ones we face. This is most clearly brought out in a comparison of Grümm's treatment of the turbulence example with the talk Dr. Bazykin gave this morning. You had in both cases a strict analogy where, by varying one parameter characterizing the behavior of your system, you move from behavior which is trivial,

concentrated in a degenerated fixed point, to behavior which is strictly periodic, to behavior which shifts the fixed point, to behavior which—though Bazykin's model did not go that far—will break down into one of these bounded but random phenomena. Dr. Bazykin obtained this result using an extremely straight forward and simple food chain model. Now we know that in other countries—I got this from discussions with Dr. Grümm—we face exactly the same sort of thing. As you vary some basic parameter such as a rate of nutrient input into a system, you move among these different types of state—space behavior: from one to another, a fixed point, a limit cycle, then converging to a more "turbulent" flow. I don't know where this sort of analyzing is going to lead, but there is clearly a parallel of sorts working here; it is going to be interesting to explore.

The other parallel notion which came out of comparison with the climatological cases is the dimensionality difficulty that comes into your models—and to the analysis technique you apply to them—brought in by spatial character of these phenomena. I agree that we can do many tricks with the local character of our processes to get the dimensionality down to such a level that many of these computational techniques can be brought to bear on them. It is not that apparent that we can do the same thing with the spatial dimension, and unless I have misread the comments from the climatologists this is a common complexity problem that neither of us has got a straightforward solution to yet. We have not been considering it as long, and we are hardly up to even their level of sophistication.

Finally, within ecology, and completely independent of particular purposes of the workshop, we have had a very good set of exchanges involving some analysis-oriented work that Rinaldi reported and a quite surprising set of developments reported by Dr. Bazykin which parallel our own studies on stability--resilience properties of these systems.

As products coming out of this workshop, I am interested in seeing whether the apparent interfacing of the differential topological views of systems behavior with techniques presently oriented towards locating fixed points—I daresay we will hear about this in methods reports that follow—whether this set of parallels is going to be further developed, here or elsewhere. As a method of integrating some of the largely static and some of them largely dynamic systems views, it sounds encouraging. The other product, on a just technical level, would be some way or other to organize the state—of—the—art techniques that have been introduced here in such a form that they are available on the IIASA or other computer systems and accessable to some of us in applied areas.

The last point is that the whole notion of stability techniques, fixed point techniques, etc., that have been touched on in this workshop sounds like potential material for a hand-book of the sort being prepared in other areas through the auspices of the Institute, here. I simply want a statement from some of the methods-people as to whether that sort of thing would be appropriate in their view. It would certainly be something which, as a user, I would find a delight to be

able to skim through. Dr. Bazykin has some comments to make. But before I give him the floor I guess I have to apologize for my scepticism in this workshop. I think a lot of us started out thinking there was a fair probability that some sort of chaos would eventually emerge from it, and I am amazed and thankful for the efforts that particularly Professor Koopmans, but also everybody here, has put into making things happen that really had no right to.

Koopmans: Thank you very much. That scepticism was beautifully concealed as far as I was concerned.

Now there were two rather distinct parts to your summary. The second of them was the point of making the state-of-the-art in computing and in formulation avaiable in some way. I would expect that there would be responses to that from methodologists. I wonder whether they would want to respond immediately. In that case, I would like to have some information as to whether Dr. Bazykin's remarks also bear on this question of computing, or whether they bear more on the questions of modeling, structures, etc. But let me first ask the methodologists. Do they want to come back to these challenges later or now?

<u>Scarf</u>: I don't quite know how one transfers state-of-the-art knowledge from one place to the other. It always seems like a terribly simple thing to do; to pick up a program and move it from point A to point B. But of course it is not that simple. Point B has to become dedicated to the use of that type of work. It is a tricky thing.

Clark: I know that IIASA is facing similar problems in some of the other handbooks being prepared here. We might not be able to write up a document on techniques which you take under your arm and go home and read it and do it. But you can discuss, not the actual operators, but, at a descriptive level, what kinds of things you can do and what you can't. What are your constraints? What are your strengths? In particular, you can start getting the names of people and some centers that are doing that kind of work. You see, as outsiders, you literally do not know where to start. Some of the books have ended up being very short things really just covering that sort of territory. I am not a handbook fan myself. The notion of working out sets of techniques as to how to do it -- which people ask you to do for ecological modeling, like everything else--has all the futility attached to it of knowing you are writing things down that you know nobody will ever read. But I think some good things can be done in that context. And, it would be nice to know what you folks think of it.

Juncosa: I can just imagine how it would work. I first try to find someone who has an interest in surveying the field. Then, several telephone conversations, communication by letters, a few spot visits in a few places, and searching for literature to put together a survey of where one stands for calculation procedures, for fixed point methods, etc. It would involve a considerable bibliography. This has been done a number of times in the history of computing, sometimes by someone who is primarily a computing person. For instance, George Forsyte's

work some 20 years ago on the solution of linear equations was widely received and an extremely valuable thing. We have to find someone who has an inclination in those directions and who will do the task. I don't think it can be done as a collective effort.

Koopmans: I now call on Dr. Bazykin.

Bazykin: My participation in the work of this workshop supported in some way my preference for further mathematical modeling in general. My first impression is trivial: the similarity of mathematical problems which arise in many distinct areas. From this point of view, I think that the efforts of those who organized the meeting of the specialists in very different areas was very good and useful. The second impression is the importance of nonlinearity in mathematical models. The main properties of nonlinear models are very distinct from the properties of the linear models, and computation of behavior of linear models is much easier. The third impression, very closely linked with the second, is that the necessity of concentrating on the integration of qualitative and simulation modeling in ecology. From my point of view the natural sequence is the following: first it is necessary to construct very simple--the simplest possible -- models of some situation, and to investigate in detail its qualitative behavior. The results of this model may lead to some idea of problems of the form of the simulation model. Those are my main impressions of the workshop.

Koopmans: As there are no questions, I call on Herb Scarf.

Scarf: I have been impressed, during this workshop, by the great difference in the ways in which various fields treat dynamic problems. I should like to make some obvious remarks about the relationship between the dynamics of the systems and the choice of a method to try to solve a particular problem.

Let me begin with some remarks about economic problems in general. We in the workshop did not get into specific details of exhibit numberical examples of economic problems that we might be interested in. We talked more about general methods than we did about the specific problems. Economics, or at least the part I am concerned with, is a rather odd field, in the sense that it is in a category where one is suspicious about the dynamics of the system. We have a notion of equilibrium, but we don't quite, at least in this field, have a clear notion about how to get there. That is, we can say when a system is not at rest; for example, if there is a very substantial demand for shoes, and a very small supply of shoes, then the system is not in equilibrium. Something will change; either the price of shoes will go up, or more shoes will be manufactured but it is not clear which of these events will take place. We recognize a disequilibrium situation but

we don't quite know the process that takes us from that disequilibrium situation to an equilibrium situation. As another example, we might look at a particular industry which has given the technical coefficients for output and the use of inputs. If that industry is making a very substantial profit, at the prices which happen to prevail, then we recognize that this system is not in equilibrium. We don't quite know however what will happen to restore an equilibrium. Will another competing organization spring into activity— will the price of the output go down? To people in the physical sciences this must seem a rather odd situation: you have a way of recognizing equilibrium and disequilibrium, but you don't quite have a story you can fully believe about the process of going from disequilibrium to equilibrium.

The problems that come to us from economics are therefore frequently in the form of: given a family of equations (not a dynamic process, but a family of equations), how to find the solutions. How to find the rest point, not what is the process for getting there. Of course, you can make a picture of this family of equations as a vector field on a sphere, and you can say that the zero of the vector field is the solution you are looking for. But it is not necessarily plausible, that the process which is obtained by following the differential equations of that vector field will correspond to the underlying economic process that takes us to equilibrium.

In this workshop we have been naturally thinking that a problem is solved by writing down a vector field and integrating the resulting differential equations. But in an economic problem the differential equations $\frac{dx}{dt} = f(x)$ can just as well be replaced by $\frac{dx}{dt}$ = Af with A an arbitrary non-singular matrix. The two systems have the same equilibrium points, but the stability properties may be quite different in the two cases. For economists it is meaningless to talk about stable points in terms of the characteristic roots of the Jacobian at equilibrium, unless we have some clear notion about the underlying dynamic process. I don't quite know whether there are other such fields, but economics can be taken as an example of the category in which dynamic problems are viewed with greater suspicion than their equilibrium counterparts. And, of course, this is the reason why fixed point methods, which are independent of considerations of local stability, play an important role in economics.

Let me contrast this approach to dynamics—where the dynamics is somewhat suspect—with a second approach to dynamics not mentioned in this workshop. Perhaps it would be appropriate to call this second category an "implicit dynamics", or "complex dynamics". What I have in mind here are problems that arise not only in economics, but physics as well, namely, where you are working with a control theory problem, or a maximization problem over time. In these problems, you are allowed to adjust a certain set of parameters subject to local constraints

at a given moment in time, in order to maximize some global objective function, which is perhaps a function of the entire path or a function of terminal conditions alone. Problems of that sort are studied in "optimal growth theory" in which resources are to be allocated over time so as to maximize global objective function. Such problems can be solved by means of the calculus of variations, or by Pontryagin's methods. It may turn out that after you have solved such a problem, the path looks as if it behaves according to some system of differential equations. But this is a derived mechanism that comes from the global problem, and is not given in advance.

I think that optimal control theory problems are an example where fixed point methods might be used in the following sense. Sometimes it is rather simple to write down explicit equations for the asymptotic state of the system. It may then be a far simpler matter to address oneself to the calculation of the stationary solution, than to calculate the entire timedependent solution starting from a given set of initial conditions. But I think it is important to recognize that in this problem the local linearization of the stationary equations may have nothing to do with the question of dynamic stability starting from a given set of initial conditions. The limiting equations are not the same thing as tracing out the path from the beginning. So again -- as in economic problems -- there is no particular point in restricting one's attention to searching for stable solutions of the limiting equations. In this sense,

control theory problems represent a case where methods which are indifferent to the question of local stability are of great importance.

Most of the problems that were discussed in this workshop fall into a third category. Namely the dynamics is simple, explicit, and described by a system of first-order differential equations. This is a case where fixed point methods have to face the simple test of whether they are any better than forward integration of the differential equation.

Charney: Only when the fixed points are stable.

Scarf: As Dr. Charney has just mentioned, one advantage of fixed point methods is that they are available even in those problems in which the equilibrium point you calculate is unstable or partially stable. I am delighted by the fact that in so many of the different applications discussed at this workshop, it does seem to be true that a search for unstable equilibrium points is of some consequence in analyzing the behavior of the dynamical system when a particular parameter is pushed beyond a certain critical level. That is, an unstable equilibrium point may indicate that a limit cycle exists in the neighborhood of this point and that time-averages of a function around the limit cycle may be approximated by the value of the function at the equilibrium point.

In the report on the paper by Eaves and myself, it was seen that the determination of a fixed point of a particular continuous mapping can be viewed as tracing out the fixed points of a homotopic family of mappings. At one extreme of

the parameter value the mapping is a trivial one with a unique fixed point which is easy to calculate. The curve of fixed points is then followed until the mapping coincides with the original mapping whose fixed point is to be determined.

It seems very possible to me that similar ideas might be useful in the calculation of limit cycles, a problem which has been identified at this workshop as being of major importance. As a homotopy parameter varies the system may pass from a stable equilibrium to a partly stable one enclosed by a limit cycle, whose calculation may be facilitated by changing the homotopy parameter in small steps.

Charney: My feeling is that probably it won't be enough to look at the unstable fixed points. We are not completely sure about that. I think in the Lorenz example it probably would have been enough to get pretty good climatology of the Lorenz-Charney model by finding all the unstable fixed points. Because they do in some sense represent good averages. If you have stable limits does that always imply that somewhere within the factor there is probably practication theory? If you have a stable limit cycle, there must also be a stable fixed point.

Rozanov: Is it possible that instead of local dynamics, but still having devised some dynamics, to put in some additional parameters which describe in some sense the ability of partners to behave? For example, you mentioned that shoe production with two possibilities: rising prices and production; so that in your model some kind of parameters are relevant to this situation, and look how your curves will be changing

if you have changed your parameters. So this approach is a very rough idea, and we don't know the dynamics, but how they are slightly changeable is not dynamics itself. I cannot formulate an equation, but do you understand what I mean?

Scarf: Yes. Economists have studied questions like this. You take a system which is in equilibrium and which has some degree of stability, and you change a parameter; e.g., a tax rate goes up, or the rate of exchange between one country and another changes, or some discovery is made of a new technical process, can you trace out the path from the old equilibrium to the new one? When the changes are small local methods are frequently adequate. Fixed point techniques were developed with the idea that sometimes large changes might be made and that the equilibrium point moves a substantial distance.

<u>Rozanov</u>: So at least it gives you the opportunity to formulate what stable or unstable means, with respect to changing of parameters. Or not exactly?

<u>Scarf</u>: Yes you could say that, but there is a distinction. For example, in Professor Molchanov's first lecture, he wrote down a system of differential equations with parameters. There was a question of whether you are concerned with stability with respect to initial states of the system, or stability with respect to the parameters as they change. I think that you are referring to stability with respect to the parameters which is stability in the sense of differential topology rather than differential equations.

Koopmans: I would like to ask for some documentation of theorems that are pertinent to the models we are discussing, and are fully covered by articles in the mathematical literature, but that are too difficult for most of the people in applied fields to read. I have two candidates for, if you like, that type of expository discussion, but there must be many more. One is a theorem by Felix Browder that deals with how the set of fixed points of a continuous mapping responds to changes in the parameters that define the mapping. It asserts a kind of semicontinuity of that set with respect to parameter changes. That would seem to me to be an important theorem for people applying these models to fully understand both the statement and the proof of. I submit the desirability of some exposition of that theorem or generalizations or specializations thereof that bear on our models.

There is also another body of theory associated with the name of Marston Morse, perhaps among others, on constellations of maxima, minima and saddle points. This could be extended I think to constellations of attractors, repellors, and other objects of the kind we are concerned with here in the workshop. Is there somewhere an expository treatment of what is known about what combinations of these objects can occur together, and which can't? It would be desirable and in some sense a mathematical contribution to the art of dynamic modeling, if we could locate such expositions if they already exist, or else induce their preparation.

<u>Scarf</u>: You have talked about two things; one is Morse theory having to do with the relationship between the characteristic roots at various zeros, but bearing only on rather special vector fields. The other has to do with fixed points of a mapping but in particular the parity of the number of fixed points. This refers to index theory in the very weakest sense, and has no dynamics associated with it. The former question is associated with the dynamics of a restricted system, and yields a global statement using much more detailed behavior at each critical point.

Koopmans: At this point I call on Dr. Juncosa.

Juncosa: Dr. Casti and I were struck by the frequency with which computing limit cycles was mentioned and many of the related problems were of the two-dimensional sort. Several people indicated that they simply integrate the differential equations for the trajectories until the trajectories appeared to be stabilizing, i.e., approaching a limit cycle.

Our feeling is that the growth of computational error in the integration of these differential equations would very frequently throw one away from the limit cycle and then one would have to approach the limit cycle anew. Thus, one may bounce back and forth and may never be really guaranteed to be close enough to the limit cycle.

For certain situations, we would like to propose a simple alternative whose originality we cannot ascertain without a search of the literature but which would avoid integration over infinitely long paths. Consider Figure 1.

Suppose that we happen to have two simple closed non-intersecting curves (K_1 and K_2 in the previous figure), one inside the other, that lie in the plane. Suppose further that, perhaps because of considerations of the orientation of the trajectories' tangent vector field, and other considerations, we know that there lies a single, stable limit cycle, L, encircling the inner closed curve K_1 and encircled by the outer one K_2 .

The proposed procedure is as follows: choose two points, A on K₁ and B on K₂ such that the line segment between them lies completely within the region between K_1 and K_2 . Starting with A and B as initial points, integrate the trajectory equations over an angle 2π) measured about A, say, from the line segment passing through A and B) to arrive at A' and B' respectively. Interpolate on the line segment (A', B') to obtain C, say, such that A'C/B'B = B'C/AA', or perhaps a different interpolation weight could be chosen. In the diagram, C is depicted inside the limit cycle L, but it could have fallen outside, depending on the interpolation. Next, integrate from C through 2π radians to get C' and interpolate with (C, C') and (B', B) between C' and B' to obtain a new point C". If C were outside the limit cycle, then (A, A') and (C, C') would be used for interpolation between A' and C' instead. The continuation is clear. nation occurs when the interpolation segment is appropriately small and consistent with the bounds in the numerical integration errors generated in the terminal integrations over 2π radians.

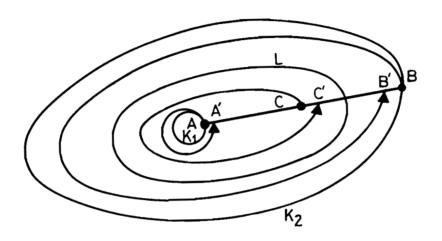


Figure 1.

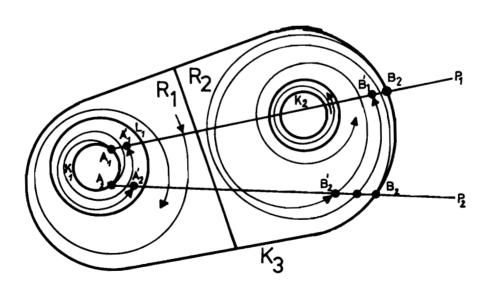


Figure 2.

If there were several limit cycles each enclosing the preceding, this process would give one of them. Search procedures would be necessary to discover the others if we did not know of their existence or non-existence a priori from other considerations.

The principal objection to an algorithm of this sort is that, as it stands, it is not totally general. For example, in other simple situations, one may have several limit cycles each inside the preceding, and, following a procedure of the above kind, one would only get one of them without any guarantee of which of the several limit cycles was obtained. Of course, further interpolatory search and integration procedures could seek out the remaining limit cycles for such a case.

If there were more than one limit cycle where one did not enclose another, more complicated problems could arise with such an approach and further research is needed here to develop a workable algorithm based on this interpolatory approach. For example, consider the following Figure 2 with two different cuts P_1 and P_2 . K_1 and K_2 are simple closed curves with outwardly flowing trajectory tangent vector fields while the field is inward on K_2 .

One can see that with the cuts P_1 and P_2 , the first point resulting from interpolation could fall in the region R_1 . This is the "fortunate" case, and the procedure described for the case of Figure 1 converges.

On the other hand, one may fall in region R_2 , the "less fortunate" case, and, clearly, we could have convergence problems. To get the limit cycle L_1 in region R_1 , we would need a rule which would stop the numerical integration when one fails after some pre-determined time to circle A with an angle of 2π with an integration that started at the point resulting from interpolation and then restart with another point closer to A than B or B'. Integration in both (x,y) and (r,θ) may be necessary to obtain stopping criteria and to shift to a new point to start the integration.

Further difficulties can arise when the cut P_2 , as distinct from P_1 does not cut the limit cycle L_2 in region R_2 ; for example, neither the second "loop" of the trajectory starting from the point B" on P_2 in R_2 nor any further "loops" of the same trajectory ever intersects P_2 again and a rule for stopping and restarting is needed.

The point to these summary remarks is that infinite integration paths may be avoided in the computation of limit cycles. In the simple cases, an algorithmic approach is given above, but for more general applications, more research is needed and a heuristic approach to develop the more general algorithms may be required.

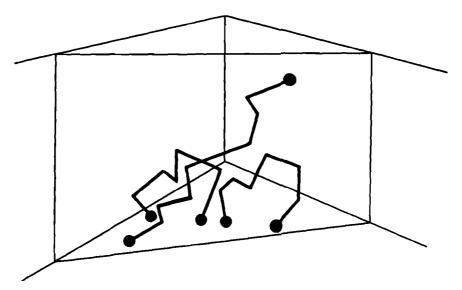
Molchanov: In particular, if someone is interested, we can offer through our computer center the Fortran Program written for such kinds of problems. Besides, we have a program which searches for Birthing Limit Cycles—a special program which automatically searches for changing of limit cycles where, depending on the parameter, it is not one system. Suppose you have a system which depends on a parameter, that program written for Fortran not only can find the limit cycle for the fixed parameter, but also they are searching for the change of the limit cycle with the change of a parameter. It is made automatically. This is dealing with three dimensions, not four. In four dimensions you might have tori. And now we are almost ready with the program for two parameters.

Koopmans: I now call on Hans Grümm.

Grümm: I would like to discuss some points in relation to the computation of closed orbits in the continuous case and periodic points in the discrete case. I would like to describe some ideas on how to combine abstract differential dynamic system results with concrete situations, to describe a cage, a region in phase space which encloses the solution (if you want to catch this rabbit you first have to put it in a cage).

In response to Dr. Juncosa, we were not unaware of the possibility of working with a Poincaré cross-section. The first problem in this approach is of course the question where to put the cross-section in a big chunk of phase space. I would like to mention two brain-bubbles that came up between Scarf and myself that can perhaps give us some guidance for further study, but certainly could not be finished during this workshop.

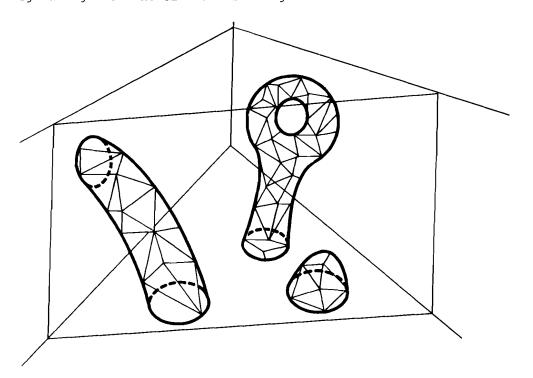
The first brain-bubble was the following. Starting with the geometric picture of the fixed point algorithms given by Eaves 1, where you have a piece-wise linear map and a piece-wise



linear situation, the pre-image under the particular map of a point is a piece-wise one-manifold, and therefore consists of piece-wise linear "segments" and "circles." In this situation you have a non-closed path starting at a fixed point and ending at a point on the boundary of the cylinder constructed by this method which is known beforehand, so that the algorithm you use would just be "retracing this path." If you could generalize this approach from a fixed point to a closed orbit, then perhaps from the closed orbit that you do not know, there would grow an inverse image of the whole orbit: a two-dimensional piece-wise linear manifold, which would then perhaps reach some boundary where you could identify its intersection and then by tracing it back, find the closed orbit. Of course you face immediately

See Scarf and Eaves, <u>The Solution of Systems of Piecewise</u> Linear Equations. (these proceedings)

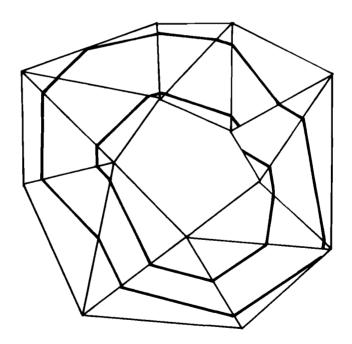
the problem of classification of two-manifolds. This is easy with one-manifolds because there are just two of them: the interval and the circle. In two dimensions, this is much more difficult, all kinds of spheres with handles occur, but the actual problem is that closed orbit might close--the two-manifold originating from the closed orbit might close onto itself. So



even if we could construct a map whose pre-image would just intersect the bottom simplex in closed orbits--better linear approximations to orbits--these pre-images might not reach the boundaries where we can trace them. The difference between the fixed point situation and this one lies in the fact that Brouwer's theorem will guarantee the existence of a fixed

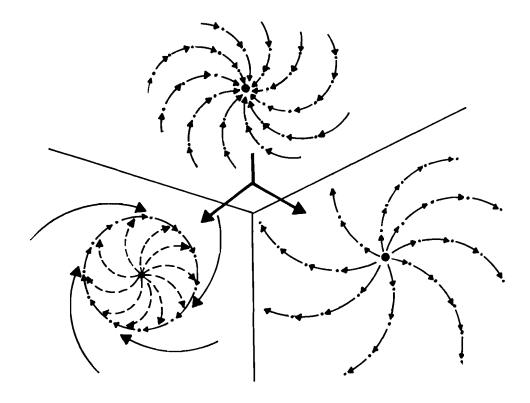
point—the path has to end somewhere—but from properties of a map at the boundaries of a simplex it is impossible to conclude the existence of a closed orbit: the homology of the simplex is trivial. To prove existence of closed orbits, you have to use toroidal (homologically non-trivial) cages.

The second idea starts with a piece-wise linear approximation of the flow (corresponding to setting the vector field constant over each subsimplex in the grid) and mapping out closed chains of simplices as in the diagram.



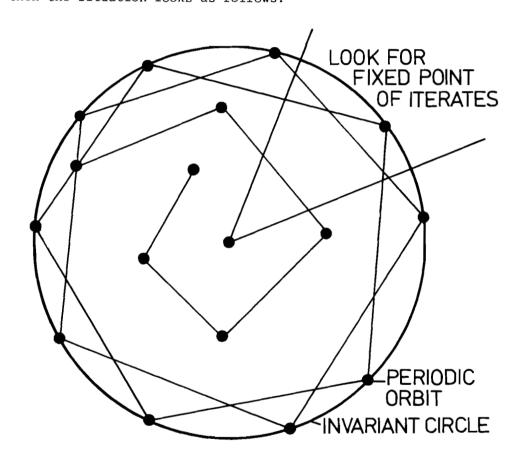
Coming back from the sky to reality, I want to make this point of a cross-section clear again. What we have learned from the whole application is the following: you have a fixed

point and some driving parameter: either some irradiation or nutrients production as in Bill Clark's trophical chain, that is slowly increased. You go on by a stable closed orbit, unstable closed orbit (but stable attracting two-torus), unstable two-torus, but stable attracting three-torus, and so on. I might state two things here. First this statement is mathematically on the level of a demonstration not of a proof. I'm using the notion that demonstrations are something that will convince a reasonable man, and a proof is something that will convince even a stubborn man. So the argument is not completely rigorous, but it is almost conclusive. The second remark that I want to make is that the same can also be done for discrete time, but here again in the vicinity of a point that has just become unstable, you will have an invariant circle, beyond that an attracting torus and so on. I would like to show you how these ideas are applied to the model Dixon Jones presented last Friday on the prey-predator situation. I would like to remind you that corresponding to the development of a certain parameter he shows the following picture: the first one with a parameter with less than a critical value; here the orbit is coming in; and in the second case he did not draw a fixed point, but everyone knew that it was there and we have some indication of where it lies. With various other points it is very unstable. So, what the Ruelle-Takens argument tells us in this particular situation is the following: you have a map with just an unstable fixed point, now you have two possibilities depending on the sign of a third order coefficient, either the orbits go away into infinity very rapidly or there is an invariant attracting circle.



Now, what does this mean in the case of discrete time; a invariant circle has nothing to do with the concept of an orbit. I might just add that while I'm drawing two-dimensional examples here, the "two" does not come from the dimensionality but just from the number of unstable eigenvalues of the Jacobian at the fixed point. So, what you are reduced to is a question of a fixed point and an attracting invariant one-manifold and now we can reduce the problem by just looking at the map restricted to this invariant circle. It might be equivalent to irrational rotations: this would certainly mean that every point starts off a dense orbit. Again I'm on the demonstration level, not on the proof level. By quoting the Peixoto theorem for the

circle which says: for an open dense subset of all differentiable systems the non-wandering set will just consist of a finite number of periodic points. If you grant me that this model will not be exceptional in this specific mathematical sense, then the situation looks as follows:



<u>Koopmans</u>: Does that have the interpretation that any point you pick will, after the finite number of successors, hit itself again?

Grümm: No, not just any point. But every point on the one-manifold will be mapped into a point on the same manifold.

<u>Koopmans</u>: Yes, but you don't necessarily go back after some iteration?

Grümm: Not necessarily, but under a genericity assumption. A finite number of points and only these points will come back to the same place after some iterations. Now, I would like to point out what goes wrong in higher dimensions. Again we find for the map an unstable circle and an attracting two-torus around it. But we don't have anything like the genericity theorem by Peixoto. In general, we will have random-like behavior on the torus and therefore in a neighborhood of it, too. Perhaps in the context of Prof. Hansen's report on the computational examples he will talk further about the details of what we did, what method we set up that still did not work.

Koopmans: There was at an earlier session a discussion which started in terms of fixed point algorithms, and then went on from calculating a fixed point by a path to estimating a closed orbit, by working in two dimensions. An expression that was used in that discussion was dropping the dimensionality in a mapping by two instead of by one. I did not recognize that idea in anything you said, but maybe it was represented.

Grdmm: It was this first idea that as a pre-image of the closed cycle, perhaps there would arise a two-manifold. Either you get the two-manifold as pre-image of a circle under a map "dropping" dimension by one, or of a point under a map dropping dimensions by two.

Koopmans: And, what is the present state of expectation for the possible feasibility and success for that procedure.

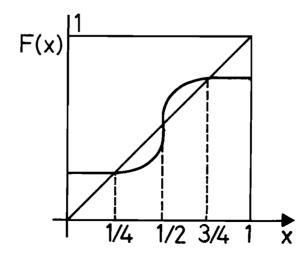
Grdmm: It is hard to say. It just occurred to me that if you know the period, you don't have to know the cross-section.

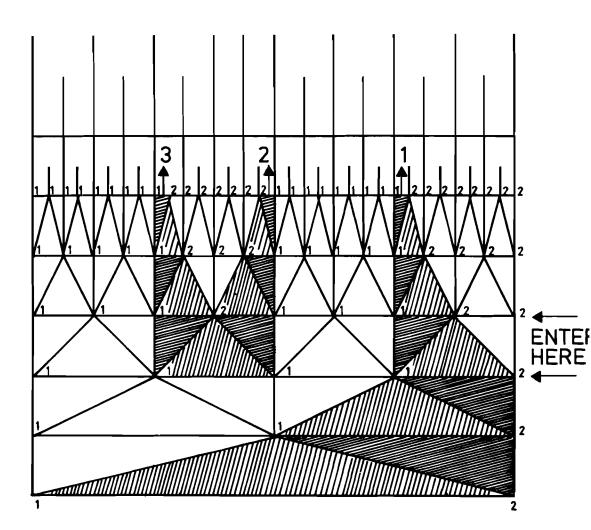
You can just make a search over the entire space to see which points are mapped into inself after this period. Iterating the map many times is just a question of computer accuracy, but not of computing time.

Koopmans: Any further questions? Then I call on Terje Hansen.

Hansen: When I came down here I had no idea what kind of problems people would be interested in doing. Conceivably we could be doing economics problems, we could be doing mathematical programming problems, we could be interested in finding a fixed point in a meteorology problem, and so on. As it turns out the interest that the people here have is somewhat different from the interest in statistical economics, where economists are typically interested in only one fixed point and, since these techniques originated in economics, the main interest so far in computational development was to make an efficient algorithm for finding one fixed point. The common characteristic of the problems that you have presented us with are that you are interested in finding many fixed points, and not only are you interested in finding many, but you are also interested in finding accurate values for many fixed points. Only the last couple of days that we have been here has it occurred to Hans Grümm and myself

that conceivably some of the techniques that have been developed for economics problems could be combined to efficiently find many fixed points. That means that then one would conceivably be able to solve with a very high degree of accuracy larger scale problems. I would like to give you an idea of this. I am limiting myself to a two-dimensional graph. There is no reason why we should not be working in n-dimensions, but this is the easier case. So, we are going to consider a trivial problem. We have a mapping of the unit simplex into itself in two-dimensions and this defines the mapping for the first variable. The function F is depicted in this graph and as you can see there are three fixed points for the map. There is one at the quarter, one at the half, and one at three quarters so we have a mapping of the unit simplex into itself with three fixed points. I just want to use this particular illustration as an example.





We are now going to consider points on the unit simplex and will associate a label with each point. The labeling rule we will use is that we associate the label "1" with a specific point, if its first coordinate is non-decreasing under the mapping. We associate label "2" if the second coordinate is non-decreasing under the mapping. So, this means in this case that we are using the label "1" in this region (pointing to the graph) and label "2" here. Note that if we take this particular problem and apply Eaves' method, which continuously refines the grid, the kind of picture we have is the following one: we are stopping the algorithm with essentially one vector where the first coordinate is zero, the second is one, another vector where the first coordinate is one, the second is zero, and a third vector where both coordinates are equal to half. Then we calculate labels. By definition all vertices, when the first coordinate is zero, are labelled "one", and all vertices, where the second coordinate is equal to zero, are labelled "two". What happens when we apply Eaves' method is that we walk up in the cylinder with continuous refinement on the grid and after several iterations we are up to a relatively fine grid. So, in this case if we apply Eaves technique we would find a fixed point that would be significant up to the sixth digit, my guess would be, if we applied something like 50 iterations. Note the problem with Eaves technique as it stands today is that it is not attuned to finding more than one fixed point. What I have done is that I have looked into the different layers here and calculated the labels for all points for the different layers

and what we see is that we have on this particular layer a point which is labeled "1" and one that is labeled "2". These two points in this case correspond to what we in the old approach called a primitive matrix, which did not work with the continuous refinement of a grid. This simplex is completely labeled so we have in this sense an approximation of a fixed point. This suggests that if we go in here (pointing to graph) on a very rough approximation, we will find completely labeled simplices, which when we put them into the Eaves diagram, will be points on an Eaves type trajectory. Thus, in this very simple example we have Eaves original trajectory going up here, which then leads us to a very good approximation of one fixed point. Then we have a funny thing coming down here, applying exactly the same kind of technique, which in this direction goies to fixed point "2", and here goes to fixed point "3".

<u>Koopmans</u>: Your "trajectory", shall I think of it as a sequence of mid-points of successive triangles?

Hansen: Yes. The thing that I want to say is that this kind of sequence of simplices, if we think in larger dimensions, goes very fast upwards such that, if we only go on to these trajectories, we could quickly get an accurate approximation of a fixed point. So, this suggests the following strategy. We try to get on the trajectory as low as possible, since the cost of getting on the trajectory depends very much on the fineness of the grid that we are applying. When we get on the trajectory we apply Eaves' technique and we get a very accurate description, a great accuracy of the fixed points.

What it means is that the kind of fixed point techniques that were originally devised by Scarf and myself, we apply to one particular level here and we make a search in order to find as many fixed points as possible. And those will then be points on the trajectories.

Koopmans: And that is all you are looking for at that level?

Grümm: You probably would only have to look for one intersection out of two intersections, of the curve of completely labeled simplices with the grid at a given level.

Hansen: Yes, but we don't know which one it is.

Grümm: OK, if I found one, I can go upwards as well as downwards.

Hansen: So, what we would do in this particular case, where we have 3 fixed points in a two-dimensional case (we have only prey, for example). We would get on a specific trajectory and then in 50 iterations for each of these trajectories (that is 55) we would have the fixed point to an accuracy of 10⁻⁶. Just to indicate some of the pitfalls that could occur in this kind of thing is that conceivably we want to get in as low as possible because that means that the research procedure is not going to be very costly. We got in here and we found that fixed point, but conceivably there could be more up here, which would then be neglected. We have a feeling that there may be some kind of connection between these trajectories. Possibly, they could be such that they were tangential to each other in the sense that we were going up here and one trajectory was more or less

fineness of grid there are some that don't get identified, and then you would have to move higher up.

<u>Jones</u>: My suggestion was that, by analogy, perhaps you could get a higher probability of picking a point on opposite sides of the fixed points with a smaller number of computations by using a random search.

<u>Hansen</u>: I think the problem is that you want to use your insight in a problem to pick the level where you want to go in and make your first search.

<u>Clark</u>: Once you decide the level of your search strategy the search can start at some regular interval, a place, random interval points, or any of the things that a normal sampling advisor would tell you to get at.

Koopmans: Can you give us some indication how you chose the horizontal level? If instead of a line segment you have the simplex in n dimensions, how do you do the search at that level or grid refinement?

Hansen: OK. Maybe I should show how this thing is done and maybe if we go to dimension 3, that would be enough to give you an idea. So, (he draws a graph on the blackboard and explains the procedure). The simplex is divided into subsimplexes. In a sense you start searching from each of the corners. Then you can start searching from the completely labled simplexes that you have found and those are the points of these trajectories that I'm referring to. The coarser the grid is the less

time it takes to get in, but the amount of points that are investigated is very small compared with the total number of vertices in the subdivision.

Schuster: I would like to ask a very brief question concerning the refinement technique. Assume you have got a completely labeled subsimplex at the level of lower accuracy. Now, your final solution need not necessarily lie inside the former subsimplex as is the case in your very simple example. For refining the grid what procedure would you suggest? In case you proceed to higher levels of accuracy and you search for completely labeled subsimplices it will occur that you do not find a solution inside your former simplex. Do you have to make a decision to go outside the given simplex or does the procedure work automatically without a particular decision of this kind?

<u>Hansen</u>: I think there is no problem. The analogy in that case is that I have searched through this grid. I have got a completely labeled simplex here. And then whatever I connect it up with there doesn't matter, because I already have all the labels represented on one grid level so the label on the next level doesn't matter.

<u>Schuster</u>: So, also in case your solution lies outside your former subsimplex the suggested procedure converges to the desired solution.

<u>Hansen</u>: It doesn't matter. The only thing that you want is to get on to this trajectory and you don't need any more information other than that you have found you need a fully labeled simplex

down here, which means that all the different labels have to occur.

I would just like to add some general comments on the ecology problem that we have been doing. In a sense we have applied the computational techniques to two classes of ecology models. One was given by Ray Hilborn and the other one is the model Dixon Jones was talking about some days ago. It seems to me that in these particular ecology models there are relatively few state variables. I don't mean 2 or 3. They are trivial, but when you get up to 5 or 6 it should be particularly suited for this kind of analysis. In both cases we then tried to find more than one fixed point. We only ran one set of parameters for each ecology model.

Bazykin: What dimension was it?

<u>Hansen</u>: The kind of techniques that we are talking about have nothing to do with dimension, so if we have a dimension 6 or 7 it doesn't matter. But the specific numerical examples only referred to 2 species and the reason is that that is the only one that they have presented. In both cases we found 3 fixed points and one, as far as I know, in your case is an unstable one and also has some particular properties.

Grümm: A fixed point generates the separatrix, the boundary between the basin of the stable equilibrium and the rest of phase space.

<u>Hansen</u>: We also tried to generate periodic points, but unfortunately we didn't get on to programming that problem until yesterday. We do not have any results to report on generating periodic points.

Molchanov: Very general case.

Hansen: There has been some misunderstanding here and what we want to do is to test a two-dimensional case because we know something of the properties of that. But the algorithm should be such that it could be done for 5, 6, 7, and 50. It should be independent of dimension.

<u>Jones</u>: Were the problems strictly computer programming ones to this point?

<u>Hansen</u>: Yes, maybe we should also say that the computer time would be in terms of 1 or 2 seconds, that would be the order of it. The problem with finding periodic points is that it would require quite considerable computer time.

<u>Jones</u>: The particular parameter set we tested was based on the visual impression of one phase diagram, which may in fact be globally unstable, so that particular set of parameters may not produce a limit cycle. But there should be some set where the periodic cycle has just been given "birth."

Grdmm: I might add that all during this workshop there has been a certain terminological confusion between the discrete and the continuous situation in this case. In this problem when we sought the solution for a periodic point, we did

not intend for this, in any sense, to be a discrete approximation. This adds another complication to the problem of the Poincaré cross-section. Why, for instance, a continuous curve or a piecewise linear or any other approximation of a curve is sure to hit this particular small piece of plane again. If you have a discrete-time system, you are moving in jumps, so you cannot hope for any particular cross-section, but just make a kind of sector so that you hope that you come back after some amount of iteration. You should not take the whole vicinity of the unstable fixed points, because for a point with a period of 20 you get 20 fixed points, which would be a terrible strain on the computer time. In a very intuitive way, there is a kind of cone where we are looking for fixed points.

<u>Scarf</u>: I think that somehow we should stay on the plane and map from the plane, say in three dimensions, to the first iteration that has just crossed the plane and then take the linear segment between the two left iterations and intersect it with the plane.

Grümm: The first return map to a plane has its particular problems when you don't know exactly how large a rotation number is going to be on the average.

Scarf: Well, but you want to avoid that by having a wedge.

<u>Hansen</u>: We have also set up the problem of chemistry; Schuster and his collaborators are looking into that right now.

<u>Schuster</u>: We succeeded in running the program of Hansen on our CDC cyber 73 computer in Vienna and tried successfully a

number of simple examples. Here I will give a short idea how fixed point techniques of the kind of Scarf's and Hansen's method can be applied to the problems we are interested in in the field of chemistry. There are two classes of problems. One kind is conventional chemical systems: we want to calculate chemical equilibria. In this case we are interested in only one fixed point and it seems to me that fixed point techniques can be applied successfully in case we rearrange our equations a little bit in order to obtain an appropriate mapping of the system on the unit simplex itself. Then with automatic grid refinement, it should be no problem to find a solution of this system of equations. We know from a physico-chemical basis that there is only one solution which makes sense.

The second kind of problem, certainly more interesting, to which I was referring here last week was the complex chemical systems, where we have to expect many fixed points. We tried one example of this kind. It was a more or less trivial test case and we obtained the correct answer. In more complicated examples one has to solve additional intrinsic equations and the program available now might in principle be applied as well. This point will be investigated further in our institute. Finally, I think, in finding fixed points in chemical systems, the technique applied here is very powerful. I would like to refer additionally to one problem which has been scratched only at the surface here. Somebody mentioned it already in the closing remarks. Up to now we have discussed more or less exclusively the evolution of our systems in time. In chemistry,

in case we are interested in unstable systems, those examples with many fixed points, we are interested also in what is going on in space. These systems show spatial instabilities as well. After passing the critical point they undergo spontaneous ordering in space. Diffusion processes are now equally important as the time development. The problem arising now is to find a solution to the system of partial differential equations. As a first step it would be desirable to approach the solution for at least one spatial variable. At the present stage of development the only approach which is applicable in general is to perform very tedious numerical integrations. What we need are more systematic investigations similar to the kind of approach we have learned about here in the case of ordinary differential equations. is just my feeling that this kind of analysis has to be extended to the case of partial differential equations in order to make the discussion gradually approaching reality. It seems to me this field is more or less open to further research.

Retrospect and Prospect

In retrospect the workshop had some of the traits of a "happening." One could not have known in advance whether the experiment of bringing together scientists from a wide range of fields on an assumption of common problems and common interests would work out. In fact, after a few days of sensing and probing, the mixture jelled. Morale, interaction and sense of valuable experience remained high from there on.

The facilities in the IIASA "Garret," with offices in which nationalities and professions were mingled like a latin square, and a central meeting room dominated by one large table and one large blackboard, fitted the purpose well. But what made the workshop was the combination of a group of scientists eager for mutual learning and a scientific situation in which such learning was found possible and regarded as fruitful.

The distribution of effort over the various activities came out differently from what had been proposed. In the minds of many of the participants, the sense of progress attached itself particularly to the use of concepts and theorems from differential topology in the description and analysis of dynamic structures. However, Professor Hansen carried the ball for computation, the ultimate purpose of the workshop activities. To express the detour taken by many other participants, the title for this Record of the Workshop is different from that by which the workshop was announced.

Measured by subjective perceptions and expressions of intellectual gain, the workshop was a success. Moreover, several participants formed plans for further collaborations. Beyond this, further evaluation of this particular effort can only be made in the future.

T.C.K.

Appendix

Papers Distributed During the Workshop

CLIMATOLOGY

- Charney, J. "On the Theory of the General Circulation of of the Atmosphere," Rossby Memorial Volume, Rockefeller Institute Press, New York, 1959, pp. 178-193.
- Lorenz, E.N. "A Study of the Predictability of a 28-Variable Atmospheric Model," <u>Tellus</u>, Vol. 3, 1965, pp. 321-333.
- Lorenz, E.N. "Climatic Change as a Mathematical Problem,"

 Journal of Applied Meteorology, Vol. 9, No. 3, June 1970,

 pp. 352-329.
- Lorenz, E.N. "Some Systems of Equations of Climate Models,"
 4 pp. These notes were made to enable participants
 to examine and select various models to try out their
 methods on.
- Lorenz, E.N. "The Mechanics of Vacillation," <u>Journal of Atmospheric Science</u>, Vol. 20, No. 5, September 1963, pp. 448-464.
- Lorenz, E.N. "The Problem of Deducing the Climate from the Governing Equations," <u>Tellus</u>, Vol. 16, No. 1, 1964, pp. 1-11.
- Phillips, N.A. "Geostrophic Motion," Reviews of Geophysics, Vol. 1, No. 2, May 1963, pp. 123-175.
- Phillips, N.A. "Models for Weather Prediction," <u>Annual</u>
 Review of Fluid Mechanics, Vol. 2, 1970, pp. 251-291.

ECOLOGY

- Gatto, M., S. Rinaldi, and C. Walters, "A Predator-Prey
 Model for Discrete-Time Commercial Fisheries,"
 IIASA Research Report (RR-75-5), March 1975.
- Holling, C.S. "Resilience and Stability of Ecological Systems," IIASA Research Report (RR-73-3), September 1973.

- Jones, D.D. "Analysis of a Compact Predator-Prey Model I.
 The Basic Equation and Behaviour," IIASA Working Paper (WP-74-34), August 1974.
- Slobodkin, L.B. "Comments from a Biologist to a Mathematician,"

 Typescript, pp. 318-329. Remarks presented at a meeting, followed by discussion.
- Slobodkin, L.B. and A. Rapoport, "An Optimal Strategy of Evolution," Quarterly Review of Biology, Vol. 49, September 1974, pp. 181-200.
- Slobodkin, L.B. and L.S.Y. Wu, "An Elementary Reconstruction of Population Dynamics," Typescript, 23 pages.

ECONOMICS

- Hansen, T. and T.C. Koopmans, "On the Definition and Computation of a Capital Stock Invariant Under Optimization," <u>Journal of Economic Theory</u>, Vol. 5, No. 3, 1972, pp. 487-523.
- Scarf, H. "An Example of an Algorithm for Calculating General Equilibrium Prices," American Fconomic Review, Vol. 59, No. 4(1), 1969, pp. 669-675.
- Shoven, J.B. and J. Whalley, "General Equilibrium with Taxes: A Computational Procedure and an Existence Proof," The Review of Economic Studies, Vol. 40, No. 4, October, 1973, pp. 475-489.

METHODS

- Casti, J. "Nonlinear Summability Methods," Prepared for the Workshop. An exposition of extrapolation methods.
- Eaves, B.C. "Properly Labeled Simplices," in G.B. Dantzig and B.C. Eaves, (ed), Studies in Optimization, Vol. 10, 1974, pp. 71-93.

- Eaves, B.C. and H. Scarf, "The Solution of Systems of Piecewise Linear Equation," Cowles Foundation Discussion Paper 390, February 1975. In part reproduced in these Proceedings.
- Kuhn, H.W. "How to Compute Economic Equilibria," January 1975. Revised text of a lecture given at Torun, Poland, July 1974. An exposition of "pivotal methods" used for the approximation of fixed points.
- Kuhn, H.W. A page from a recent letter from Kuhn and a brief memo modifying the statements in the above text with regard to sizes of problems that can be handled. References in the memo to pages and problem types refer to the above lecture.
- Robinson, S.M. "Newton's Method for Systems of Non-linear Equations," <u>Typescript</u>, 6 pages, prepared for the Workshop. Included in these Proceedings.
- Scarf, H. Introduction to a book containing papers delivered at a symposium on fixed-point methods, presented at Clemson University in the spring of 1974.

