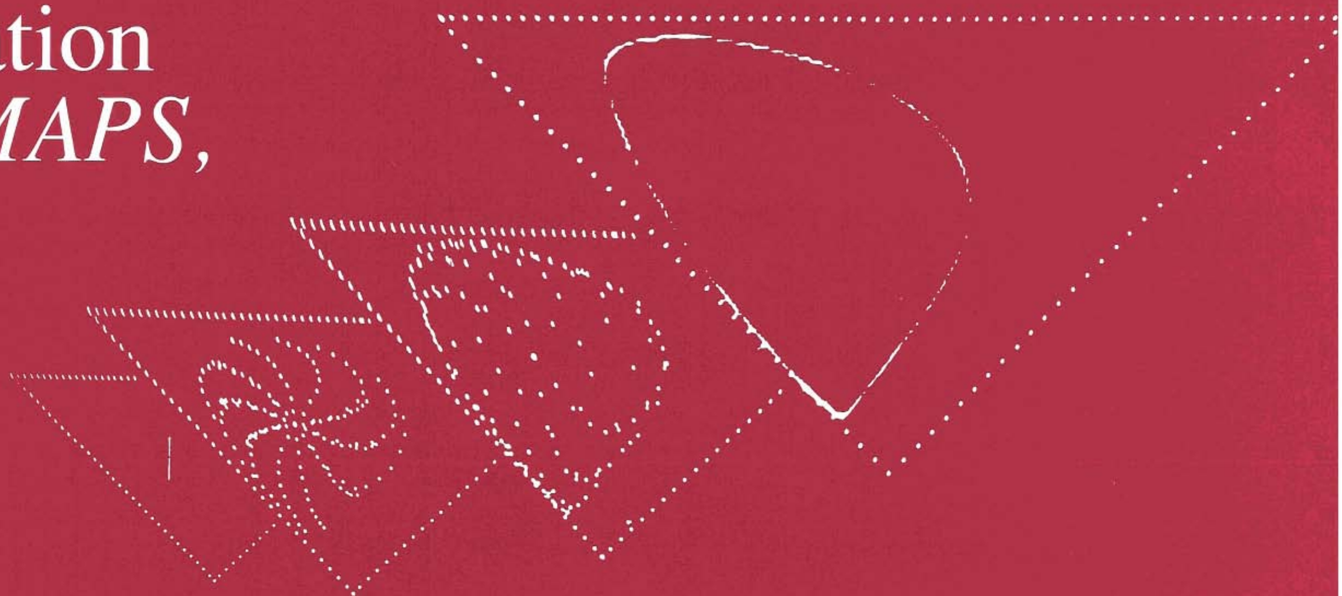
Iteration of *MAPS*,



STRANGE ATTRACTORS, and *NUMBER THEORY*

— *AN ULAMIAN POTPOURRI*

by *Paul R. Stein*

I first met Stan Ulam during the war, when I was at Los Alamos as a GI, working in Hans Bethe's Theoretical Division. Our friendship was social rather than professional, for at that time I had little to contribute. I returned to Los Alamos in 1950 and was immediately caught up in the weapons program, spending much of my time in the East helping to run problems on computers in Washington, Philadelphia, and Aberdeen. What time remained was spent in Santa Monica consulting with the Rand Corporation—and courting my future wife. Fortunately, in 1953 I managed to get married, and that, of course, settled me down. The next six years witnessed my gradual conversion, under Stan's tutelage, from physicist to mathematician.

Our collaboration started in a low key. At first it was limited to discussions—rather one-sided, as I recall. I listened as Stan aired his prejudices concerning mathematical biology as it then was (circa 1955): "It is all foolishness, don't you think?" I was in no position to counter these remarks, and soon he had me more or less believing them. One argument he advanced more than once (and which I no longer believe) was about the human eye. Stan could not imagine that something so complex could have evolved by random processes in the time available, even granting the effect of natural selection. Neither of us, however, could think of a practicable calculation to settle the question, so we turned to simpler matters.

The first mathematical problem we undertook together, with the aid of an IBM 704 computer, concerned the evolution of large populations under the assumption of random mating, to which we added the effect of mutation. (This description of the problem may tempt the reader to interpret what follows in terms of Mendelian genetics. That topic, however, had already been treated mathematically in great detail, and our interest lay rather in investigating mathematical and computational approaches to other examples of evolutionary processes.) Stan made it very clear that he wanted nothing to do with the customary approach via differential equations (à la Sewall Wright); instead, everything was to be based on point-wise iteration. I heartily agreed.

We characterized the "type" of an individual in the population by a pair of integer indices (i,j), with $i,j = 1,2,\ldots,N$. The number of males of type (i,j) was assumed to equal the number of females of that type; in fact, males and females were not distinguished, so, despite the use of the word "mating," the problem involved no sex (and none of the mathematical complications that go with it). The fraction of individuals of type (i,j) in the nth generation of the population was denoted by $x_{ij}^{(n)} = x_{ji}^{(n)}$. Random mating then changes the population fractions from generation to generation according to the equation

$$x_{ij}^{(n+1)} = \sum_{p,q,r,s} \gamma_i^{pr} \gamma_j^{qs} x_{pq}^{(n)} x_{rs}^{(n)}. \tag{1}$$

The summation in Eq. 1 was carried out under the restrictions of a "mating rule," namely, that progeny of type (i,j) result from mating between individuals of type (p,q) and (r,s) only if

$$\min(p,r) \le i \le \max(p,r)$$

and

$$\min(q,s) \le j \le \max(q,s). \tag{2}$$

(Here $\min(u,v)$ and $\max(u,v)$ mean, respectively, the smaller and the larger of the two integers u and v.) In other words, the indices of an offspring fall within the ranges defined by those of its parents.

For technical reasons that I will not pursue here, we imposed simplifying conditions on the coefficients γ_k^{uv} as follows:

$$\begin{aligned} \gamma_k^{uv} = \gamma_k^{vu} &> 0 \quad \text{if } \min(u,v) \le k \le \max(u,v), \\ &= 0 \quad \text{otherwise (in conformance with the mating rule);} \end{aligned} \tag{3}$$

$$\sum_{k=v}^{u} \gamma_k^{uv} = 1; \tag{4}$$

and

$$\sum_{k=v}^{u} k\, \gamma_k^{uv} = \frac{u+v}{2}. \tag{5}$$

Finally, we normalized the initial population fractions $x_{ij}^{(0)}$ by requiring that

$$\sum_{i,j=1}^{N} x_{ij}^{(0)} = 1. \tag{6}$$

It is easy to show that the normalization is preserved through all generations, or in other words that

$$\sum_{i,j=1}^{N} x_{ij}^{(n)} = 1 \quad \text{for all } n.$$

To include mutation we modified Eq. 1 by adding linear terms multiplied by a small positive number ϵ:

$$x_{ij}^{(n+1)} = -\epsilon x_{ij}^{(n)} + \frac{\epsilon}{2}\left(x_{i-1,j}^{(n)} + x_{i,j-1}^{(n)}\right) + \sum_{p,q,r,s} \gamma_i^{pr} \gamma_j^{qs} x_{pq}^{(n)} x_{rs}^{(n)}. \tag{7}$$

(The added terms reflect the assumption that mutation causes type (u, v) to give rise to types $(u+1, v)$ and $(u, v+1)$ with probability $\frac{1}{2}\epsilon$.)

We performed very many numerical experiments on the systems represented by Eq. 7, varying ϵ and using special sets of coefficients satisfying Eqs. 3, 4, and 5. Two particularly convenient coefficient sets were

$$\gamma_i^{jk} = \frac{1}{2^{|j-k|}} \binom{|j-k|}{i - \min(j,k)}$$

(where the term in parentheses is the usual binomial coefficient) and

$$\gamma_i^{jk} = \frac{1}{|j-k|+1}.$$

Unfortunately, the detailed results of these experiments have disappeared over the thirty or so years since the computations were done. I seem to recall, however, that all the systems we looked at "converged"; in fact, after a sufficiently large number of generations, only a single type remained (survival of the fittest?). I also remember that the convergence was not usually monotone.

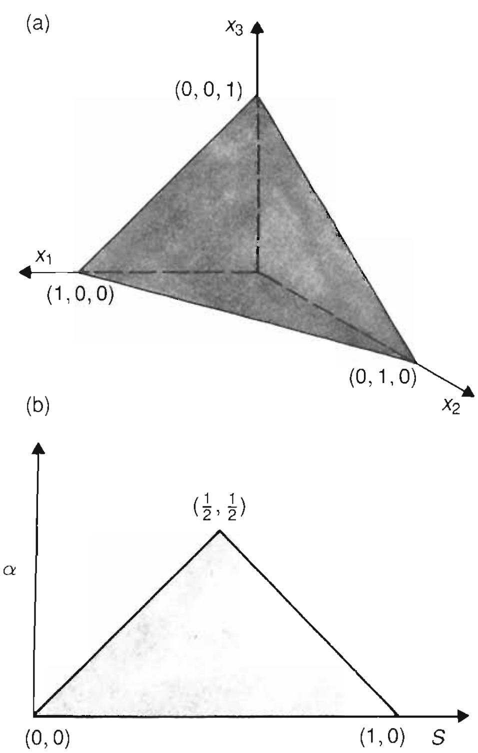
Although nothing of a detailed theoretical nature was discovered about the systems including mutation, the simpler systems without mutation (Eq. 1) could be analyzed exactly by elementary methods, even when individuals were distinguished by many indices rather than only two. In brief, each system, as defined by a set of initial population fractions, converged to a state determined entirely by that set. (Details of the analysis are given in Menzel, Stein, and Ulam 1959 and in Stein and Ulam 1964.)

Our next joint project was undertaken with more mathematical aims in view, although Stan never lost his strong interest in biology. (A good summary of Stan's contributions to that field can be found in a 1985 article by Beyer, Sellers, and Waterman. The reader should take note of the 1967 paper by Schrandt and Ulam. The study of growth patterns contained therein bears a close resemblance to some recent work on cellular automata.) After extensive discussion, we decided to study the behavior under iteration of a restricted class of quadratic transformations, or maps, of the plane. The idea was mainly Stan's, but I managed to contribute some practical suggestions.

At this point is seems appropriate to explain what it meant to collaborate with Stan. At some stage in his mathematical career, he apparently lost his taste for detailed mathematical work. Of course, his mind was always brimmming with ideas, most

DOMAIN OF TWO-DIMENSIONAL MAPS

Fig. 1. The restrictions $0 \leq x_i \leq 1$ (i = 1, 2, 3) and $\sum_1^3 x_i = 1$ limit the domain of the x_i's, and of the iterates of the two-dimensional quadratic and cubic maps discussed in the text, to the equilateral triangle shown in (a). For more convenient graphic display of the iterates, we introduced the variables $S = \frac{1}{2}(1 + x_1 - x_3)$ and $\alpha = \frac{1}{2}x_2 = \frac{1}{2}(1 - x_1 - x_3)$. These new variables, and the iterates of the maps, are limited (by the restrictions on the x_i's) to the isosceles triangle shown in (b).



of them good; it was the collaborator's job to fill in the details. Stan was often of great help here with suggestions on how to evade difficulties, but he himself would not work out anything that required more than a few lines of calculation. In the late 1940s C. J. Everett and Stan wrote three brilliant papers on branching processes in n dimensions—a technical tour de force. I recently asked Everett how he and Stan had worked together on those papers. Everett's reply was succinct: "Ulam told me what to do, and I did it." In my case collaboration with Stan usually involved a third person. I had given up programming after having had my fill of it during the first three years at Los Alamos. (In the last four years I have had to take it up again.) Among those who did my coding from time to time were Bob Bivins, Cerda Evans, Verna Gardiner, Mary Menzel, Dorothy Williamson, and in particular Myron Stein, who collaborated with me for many years until the pressure of his own work made it impossible.

The study Stan and I made of quadratic transformations used the programming skills of Mary Menzel; the results appeared in 1959 as "Quadratic Transformations, Part I"—there never was a Part II—under all three names. The computations were done on the Laboratory's own computer, MANIAC II (now defunct). In the following section I will describe that study in some detail; it will then be unnecessary to say much about the mechanical aspects of our later (and more exciting) generalization to cubic maps, since the underlying assumptions were the same.

Quadratic Transformations à la Stein-Ulam

Consider three variables x_1, x_2, and x_3 restricted as follows:

$$0 \leq x_i \leq 1, \quad i = 1, 2, 3$$

and

$$x_1 + x_2 + x_3 = 1. \tag{8}$$

These restrictions limit the variables to the two-dimensional domain shown in Fig. 1a.

If we multiply out $(x_1 + x_2 + x_3)^2$, we get the six terms x_1^2, x_2^2, x_3^2, $2x_1x_2$, $2x_1x_3$, and $2x_2x_3$. We distribute these six terms among three nonidentical boxes, no box remaining empty. (The boxes correspond to the transformed variables x_1', x_2', and x_3'.) This distribution can be done in many ways, in fact, in 540 ways. (The distribution (4,1,1), that is, the distribution such that the first box contains four terms and the second and third boxes each contain one term, can be done in thirty ways, as can the distributions (1,4,1) and (1,1,4); the distributions (3,2,1), (3,1,2), (1,3,2), (1,2,3), (2,1,3), and (2,3,1) each in sixty ways; and the distribution (2,2,2) in ninety.) Let us choose the distribution (3,2,1) to construct an example of a quadratic map. We take three terms, say x_1^2, $2x_1x_2$, and $2x_2x_3$, and form their sum; then we sum two other terms, say x_2^2 and x_3^2, leaving the term $2x_1x_3$ to stand alone. The corresponding map is given by the equations

$$\begin{aligned} x_1' &= x_1^2 + 2x_1x_2 + 2x_2x_3 \\ x_2' &= x_2^2 + x_3^2 \\ x_3' &= 2x_1x_3. \end{aligned} \tag{9}$$

Iteration is carried out by setting x_i equal to x_i' (the first iterate) and substituting the new x_i's back into the right side of Eq. 9 ad infinitum.

Biology has not quite disappeared from the problem. If the x_i's are interpreted as population fractions, Eq. 9 represents the evolution of a population containing three types of individuals randomly mating according to the following rule:

> mating between types 1 and 1, 1 and 2, and 2 and 3 produces type 1;
> mating between types 2 and 2 and 3 and 3 produces type 2;
> and mating between types 1 and 3 produces type 3.

One could also write this rule as a table or a matrix, forms that are more revealing of the algebraic and group properties of the transformation.

Note that if we add up the three rows of Eq. 9, we get $x_1'+x_2'+x_3' = (x_1+x_2+x_3)^2$, which equals unity because of Eq. 8. Thus the normalization is preserved algebraically. Nevertheless, in carrying out the iterations on MANIAC II we found that D, the sum of the computed x_i''s, could be slightly different from unity because of roundoff. Therefore it was necessary to renormalize after each iteration as follows: $x_i'/D \rightarrow x_i'$ for all i.

The "fixed points" of a transformation (more precisely the "first-order fixed points") are points that remain unchanged under iteration; they are solutions to the equations obtained by removing the primes on the equations defining the transformation. The fixed points for the map given by Eq. 9 are easily determined. First note that $x_3 = 2x_1x_3$ (obtained from the third row of Eq. 9) implies that $x_3 = 0$ or $x_1 = \frac{1}{2}$. These possibilities, together with $x_1 = x_1^2 + 2x_1x_2 + 2x_2x_3$ (obtained from the first row of Eq. 9) and the restriction $x_1+x_2+x_3 = 1$, lead to two "nodal" fixed points, (1,0,0) and (0,1,0), and one "internal" fixed point, $\left(\frac{1}{2}, \frac{1}{4}(2-\sqrt{2}), \frac{1}{4}\sqrt{2}\right)$.

How does the map given by Eq. 9 behave under iteration? Experimentally, if we choose an initial point (x_1, x_2, x_3) at random, it is highly probable that the successive iterates will converge to the map's internal fixed point. For some initial points, including those such that $x_3 = 0$ and $x_1 \neq 0$, the iterates converge to the nodal fixed point (1,0,0). (The other nodal fixed point is nonattractive: iterates diverge from (0,1,0) no matter how close to that point an initial point may be.) So this map has two attractive limit sets, or attractors, each characterized by its "basin of attraction" (the set of initial points that iterate to the attractor).

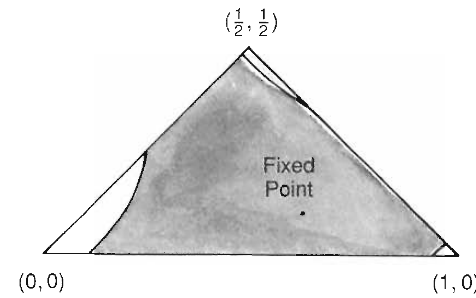
As mentioned above, there are many more maps of the present kind, which we called binary reaction systems. Fortunately, we needed to examine only those that are inequivalent, that is, those that cannot be transformed into each other by some permutation of the indices on the x_i's and the x_i''s (the order of the rows clearly does not matter). It turns out that precisely 97 of the possible 540 maps are inequivalent according to this criterion. The fixed points of all the inequivalent maps were worked out by hand (Stan himself verified some of those calculations), and their limiting behavior under iteration from several randomly chosen initial points was examined numerically. The latter was a very slow process in 1958: MANIAC II could perform only about fifty such iterations per second. Of course, MANIAC II was a stand-alone "dedicated" machine, and that helped make up for its lack of speed.

For more convenient graphic display of the results, we arbitrarily introduced two new variables

$$S = \frac{1}{2}(1 + x_1 - x_3) \text{ and } \alpha = \frac{1}{2}x_2 = \frac{1}{2}(1 - x_1 - x_3). \tag{10}$$

DEPENDENCE OF LIMIT SET ON INITIAL POINT OF ITERATION

Fig. 2. A few of our two-dimensional quadratic maps exhibited one of two limiting behaviors under iteration, depending on the location of the initial point. For example, the map defined by the equations below (in both x_i and S, α coordinates) iterates to an internal fixed point (S_0 = 0.62448516, α_0 = 0.09239627) from any initial point within the dark gray region of the reference triangle and to a nodal period of order 3 $\left((0,0) \rightarrow (\frac{1}{2},\frac{1}{2}) \rightarrow (1,0)\right)$ from any initial point within any of the three light gray regions. The "separatrix" demarcating the basins of attraction of the two limit sets was determined experimentally.



$$T_{x_i}: \begin{aligned} x_1' &= x_2^2 + 2x_1x_2 + 2x_1x_3 \\ x_2' &= x_3^2 + 2x_2x_3 \\ x_3' &= x_1^2 \end{aligned}$$

$$T_{S,\alpha}: \begin{aligned} S' &= \frac{1}{2}(1 + \alpha^2 - 3S^2) - \alpha + S + 3\alpha S \\ \alpha' &= \frac{1}{2}(1 + S^2 - 3\alpha^2) + \alpha - S - \alpha S \end{aligned}$$

The domain of these new variables is an isosceles triangle in the S, α plane, with unit base and half-unit height (Fig. 1b). Note that the vertices of this "reference triangle" correspond to the nodal points of the original domain.

What we found was less than overwhelming. One transformation had an internal periodic limit set of order 3 (that is, its limit set consisted of three internal points traversed in a certain order), four had internal periods of order 2, one showed no limiting behavior at all, and one converged to an internal fixed point as $\frac{1}{r}$, where r is the distance of the iterate from the fixed point. In addition, a few maps had a "separatrix" (Fig. 2); that is, they showed one of two limiting behaviors (usually convergence to a fixed point or to a periodic limit set of order 2) depending on the location of the initial point. Everything else converged to a fixed point (not necessarily internal) or had nodal periods of order 2 or 3. The interested reader will find a description of the many generalizations we tried in Menzel, Stein, and Ulam 1959.

Cubic Maps and Chaos

Although some interesting facts emerged from the study described above, Stan and I were disappointed at the lack of variety in the limiting behavior we observed. We even tried to enliven the situation by generalizing the generic map to the form

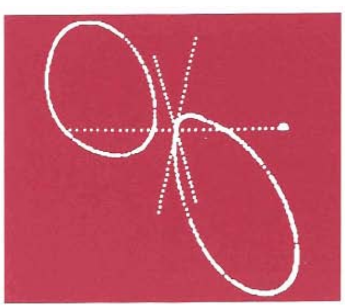
$$x_i' = d_{i1}x_1^2 + d_{i2}x_2^2 + d_{i3}x_3^2 + 2d_{i4}x_1x_2 + 2d_{i5}x_1x_3 + 2d_{i6}x_2x_3, \quad i = 1,2,3,$$

with the coefficients randomly chosen but restricted by $0 \le d_{ij} \le 1$ for all i,j and $\sum_{i=1}^{3} d_{ij} = 1$. Of several hundred such systems investigated, almost all iterated to a fixed point; in other words, the special quadratic maps we had originally looked at were more interesting than the general case.

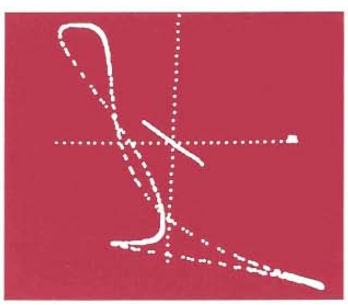
What to do? Stan and I had, simultaneously, the idea of looking at three-variable cubic maps of the same structure as our quadratics. That is, we would distribute the ten terms arising from expansion of $(x_1 + x_2 + x_3)^3$ among three boxes and construct the maps in the same way as before. A short calculation (see pp. 7–8 of Stein and Ulam 1964) showed that there were more than 9330 inequivalent maps of this type. (The

THREE-DIMENSIONAL QUADRATIC MAPS WITH INFINITE LIMIT SETS

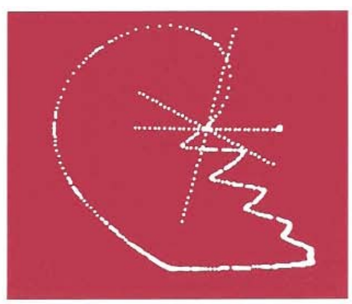
Fig. 3. The limit sets of a small fraction of our quadratic transformations in four variables contain what appear to be infinite numbers of points. Shown below are three-dimensional projections of four such limit sets, which were obtained by photographing plots of successive iterates on an oscilloscope screen. The set of axes in the center of each display indicates the orientation of the limit set relative to the viewer, who is conceived of as stationed at a certain distance from the origin along the x_2 axis. The limit set for T_a consists of two "curves," one in the x_1, x_3 plane and the other in a plane inclined at 45° to the x_1, x_3 plane. T_a evidently transforms these planes into each other, since successive iterates lie alternately on the two curves. The limit sets for T_b, T_c, and T_d are even more complicated, constituting implausibly tortuous curves in space.



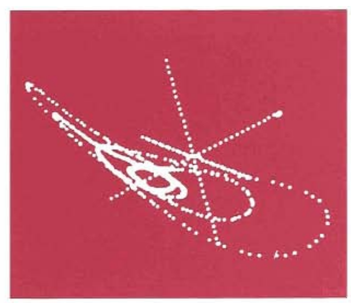
$$T_a: \begin{aligned} x_1' &= x_1^2 + x_2^2 + 2x_2x_4 \\ x_2' &= x_4^2 + 2x_1x_4 + 2x_3x_4 \\ x_3' &= x_3^2 + 2x_1x_2 + 2x_1x_3 \\ x_4' &= 2x_2x_3 \end{aligned}$$



$$T_b: \begin{aligned} x_1' &= x_1^2 + x_3^2 + 2x_3x_4 \\ x_2' &= x_4^2 + 2x_1x_4 + 2x_2x_4 \\ x_3' &= x_2^2 + 2x_1x_2 \\ x_4' &= 2x_1x_3 + 2x_2x_3 \end{aligned}$$



$$T_c: \begin{aligned} x_1' &= x_1^2 + x_3^2 + 2x_1x_2 \\ x_2' &= 2x_1x_3 + 2x_2x_4 + 2x_3x_4 \\ x_3' &= x_2^2 + 2x_2x_3 \\ x_4' &= x_4^2 + 2x_1x_4 \end{aligned}$$



$$T_d: \begin{aligned} x_1' &= x_1^2 + 2x_1x_4 + 2x_2x_4 \\ x_2' &= x_3^2 + x_4^2 + 2x_2x_3 \\ x_3' &= x_2^2 + 2x_1x_2 + 2x_3x_4 \\ x_4' &= 2x_1x_3 \end{aligned}$$

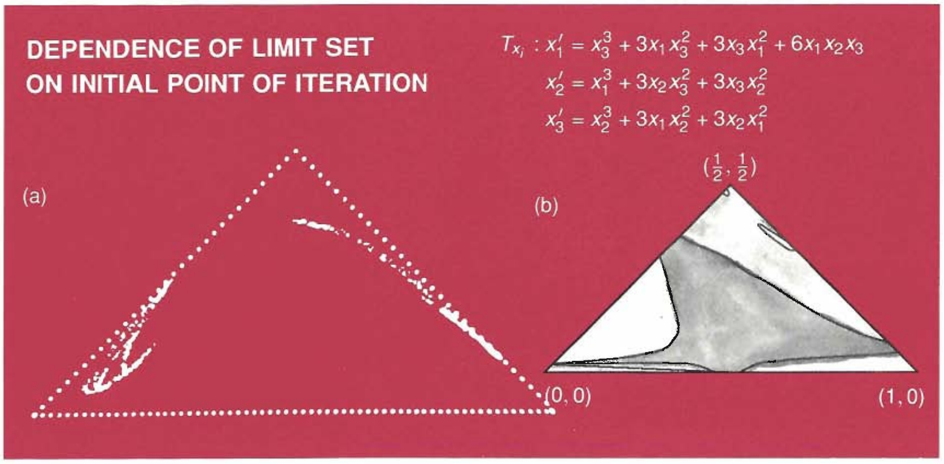


Fig. 4. Shown in (a) is one of two possible limiting behaviors for the map defined by the given equations, namely, convergence to a "mess," an apparently infinite number of points with a complex distribution and no discernible structure. The map iterates to this messy limit set from any initial point within any of the light gray regions in (b). If, however, the initial point lies within any of the dark gray regions, the map iterates to the fixed point $S_0 = 0.6259977$, $\alpha_0 = 0.1107896$. The complicated separatrix was determined experimentally.

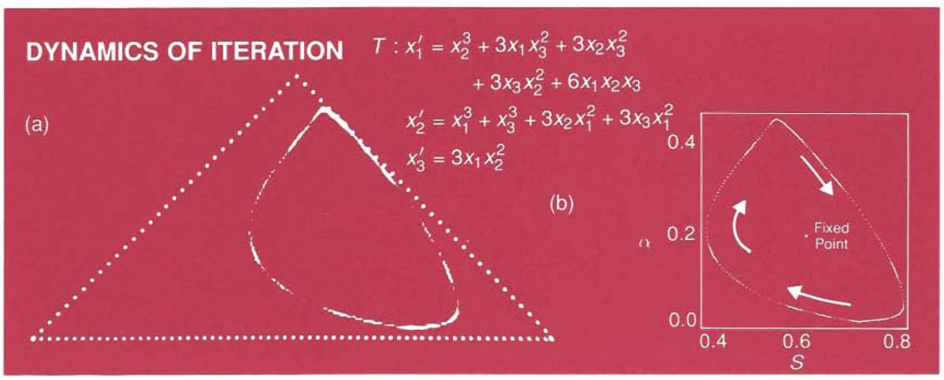


Fig. 5. The two-dimensional cubic map defined by the given equations iterates to an infinite limit set composing the closed curve shown in (a). (Whether the words "infinite" and "curve" can be applied here in the strict mathematical sense is not known.) When this map is iterated from some point p in the limit set, successive iterates do not trace out the curve in an orderly fashion. However, the 71st, 142nd, 213th, . . . , $(71n)$th, . . . iterates of p, which are plotted in (b), do lie close to each other and trace out the curve in a clockwise direction. Various stages in the iteration of this map are featured in the art work on the opening page of the article. The first image (counted from background to foreground) shows the set of points at which the iterations were begun, namely twenty-one points uniformly distributed along a line segment whose midpoint is coincident with the nonattractive fixed point of the transformation. (The horizontal and vertical coordinates of this fixed point are approximately 0.6149 and 0.1944, respectively.) The second and third images, which are superpositions of the 8th through 15th and the 15th through 22nd sets of iterates, respectively, capture the dynamics of these early iterations. The final image, a superposition of the 1800th through 2700th sets of iterates (and the same as that in (a) here), shows the stable pattern to which the sets of iterates converge.

exact number turned out to be 9370, arrived at by a more complicated combinatorial calculation.) Perhaps among this plethora of possibilities we would find some systems that showed truly unexpected limiting behavior. I am happy to say that the results far exceeded our expectations.

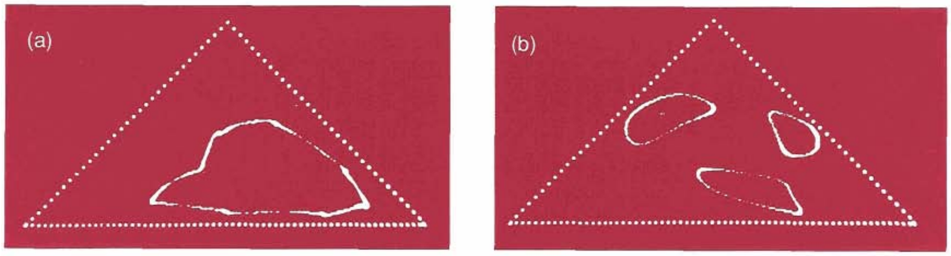
We also considered transformation in three dimensions, specifically quadratics in four variables with $x_1 + x_2 + x_3 + x_4 = 1$. But 34,337 of these are inequivalent (not an easy fact to come by), so we were never able to give them the attention they deserved. (Figure 3 gives a glimpse of some interesting cases.) Unless someone writes a fast program to evaluate automatically the amusement value of limit sets, that is as far as such studies will ever go: the case that comes next (when ranked by the number of inequivalent maps) is that of quartics in three variables, and more than 3,275,101 of these are inequivalent (the exact number is unknown).

Returning to our study of cubic maps, we plotted the sets of points obtained by iteration on an oscilloscope screen in the reference triangle of Fig. 1b. "Hard copy" was obtained directly from the screen with a Polaroid camera mounted on the oscilloscope. This method, in addition to being cheaper, was more convenient than the current method, which involves a \$20,000 Tektronix terminal with a hard-copy device.

There is not enough space to give all the details of what we found; an extensive summary is given in Stein and Ulam 1964, and Figs. 4–7 show some interesting

TWO AMUSING INFINITE LIMIT SETS

Fig. 6. Examples of two-dimensional cubic maps with infinite limit sets constituting (a) a more irregular closed curve than that illustrated in Fig. 5 and (b) three separate closed curves.

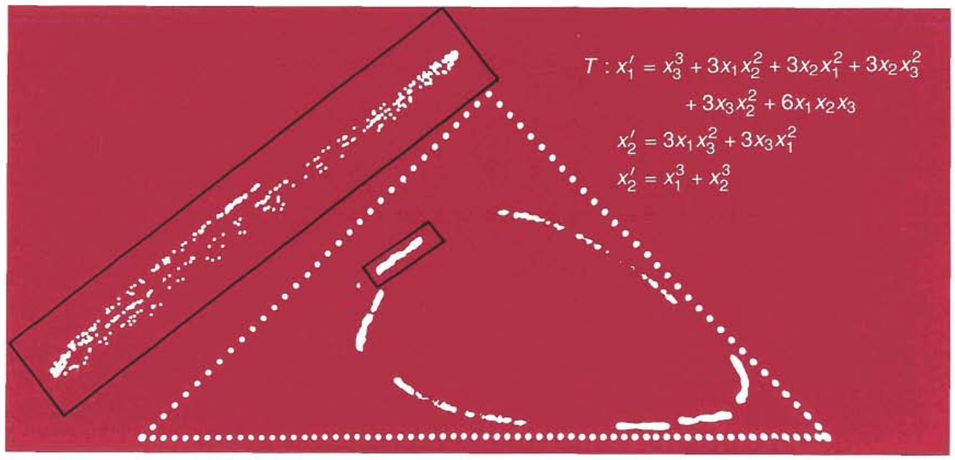


$$T_a : x_1' = x_1^3 + x_2^3 + x_3^3 + 3x_1x_2^2 + 3x_2x_1^2$$
$$x_2' = 3x_2x_3^2 + 3x_3x_2^2 + 6x_1x_2x_3$$
$$x_3' = 3x_1x_3^2 + 3x_3x_1^2$$

$$T_b : x_1' = 3x_1x_3^2 + 3x_2x_3^2 + 3x_3x_1^2 + 3x_3x_2^2$$
$$x_2' = x_1^3 + 3x_2x_1^2 + 6x_1x_2x_3$$
$$x_2' = x_2^3 + x_3^3 + 3x_1x_2^2$$

A PARTICULARLY FASCINATING INFINITE LIMIT SET

Fig. 7. The infinite limit set of the two-dimensional cubic map defined here consists of seven separate subsets. Each subset is invariant under the seventh power of the transformation; that is, if p is a point in any one of the subsets, the 7th, 14th, 21st, . . . , (7n)th, . . . iterates of p are also in that subset. Shown magnified in the inset are the 7th, 14th, 21st, . . . , 2695th iterates of a point in the outlined subset of the limit set.



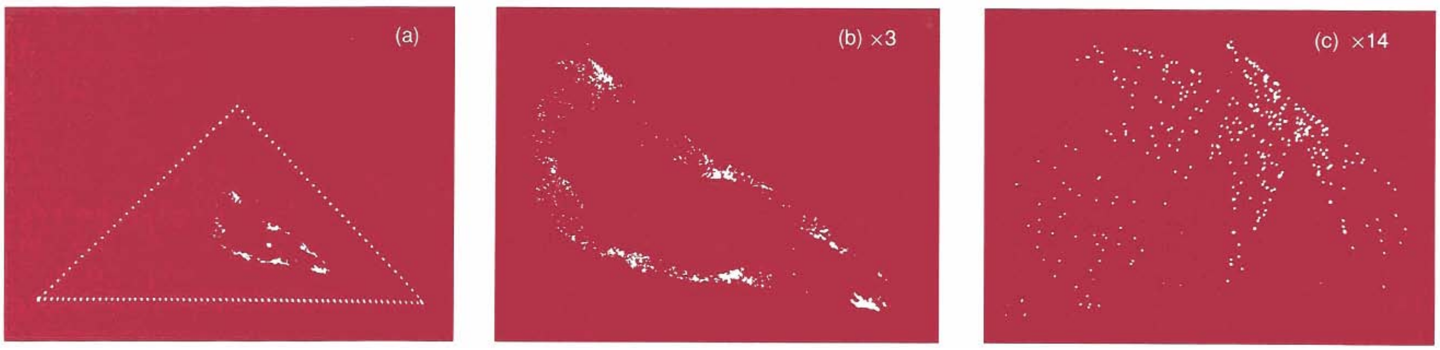
examples of limiting behavior. Again, a large majority of the transformations converged to fixed points or to periodic limit sets (some of quite high order). Of most interest to us, however, were 334 transformations that exhibited no periodic limiting behavior, suggesting that their limit sets contained infinite numbers of points. Some of these appeared to be closed curves or sets of closed curves, although to this day not one has been shown to satisfy the mathematical criteria for a curve. Others bore a striking resemblance to the night sky; at the time these strange limit sets were commonly referred to as messes.

The transformation that iterated to the mess shown in Fig. 8 was studied in great detail and received the special name T_{A}. For the record I give its definition here, both in x_i and S, α coordinates.

$$\begin{aligned} T_{\mathrm{A}} : x_1' &= x_3^3 + 3x_1x_3^2 + 3x_2x_3^2 + 3x_3x_2^2 + 6x_1x_2x_3 \\ x_2' &= x_1^3 + x_2^3 + 3x_3x_1^2 \\ x_3' &= 3x_1x_2^2 + 3x_2x_1^2 \end{aligned} \tag{11a}$$

and

$$\begin{aligned} T_{\mathrm{A}} : S' &= S^3 - 6S^2\alpha - 3S\alpha^2 + 4\alpha^3 - \frac{3}{2}S^2 + 3S\alpha - \frac{3}{2}\alpha^2 + 1 \\ \alpha' &= -S^3 + 3S\alpha^2 + 2\alpha^3 + \frac{3}{2}S^2 - 3S\alpha + \frac{3}{2}\alpha^2. \end{aligned} \tag{11b}$$



THE INFINITE LIMIT SET OF T_A—A "MESS"

Fig. 8. The transformation T_A (see text for defining equations) is one of our two-dimensional cubic maps that iterates to a mess. Shown in (a) is its messy limit set; its nonattractive fixed point has been superimposed on the photograph. The magnifications in (b) and (c) reveal ever greater complexities.

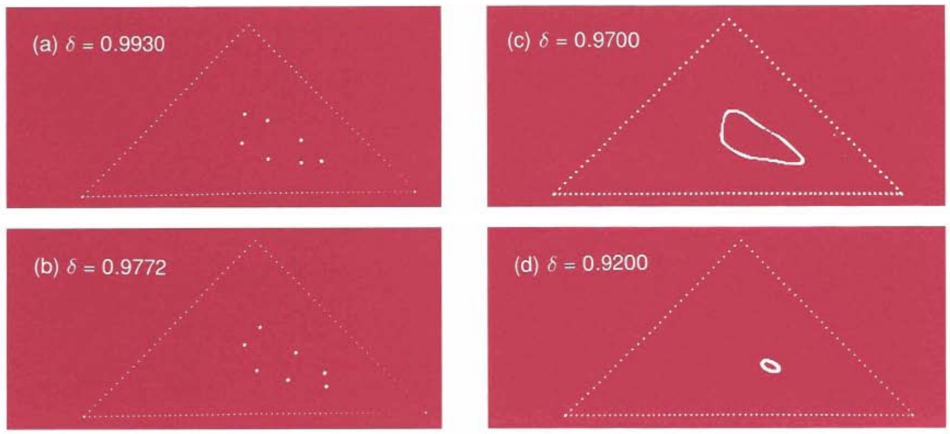
T_A has an unstable (nonattractive) internal fixed point; its approximate coordinates are $S_0 = 0.5885696$ and $\alpha_0 = 0.1388662$. Some twenty years after the appearance of our paper, T_A was examined on a Cray computer by Erica Jen. The results strongly suggested that its limit set is what is today called a strange attractor, with a fractal (noninteger) dimension of about 1.7. The term "strange attractor" was coined by Ruelle and Takens in 1971 in the course of a study of turbulence. Strange attractors are now known to arise often during iteration of the nonlinear differential or difference equations used to describe phenomena in, for example, meteorology and fluid dynamics.

Several other messes have been classified as strange attractors by present-day criteria, the main one being sensitive dependence on initial conditions. That is, a limit set is a strange attractor if any two points within the set, no matter how close, move farther and farther apart under the action of the mapping. If the limit set is bounded away from infinity (as it is here), the points cannot keep moving apart, and the criterion then is that the relative positions of the limit points become uncorrelated—a feature of chaos. Unfortunately, no numerical experiment can *prove* that some limit set is a strange attractor. For example, what appears to be a strange attractor may actually be a periodic limit set of very high order. To my knowledge, rigorous measures of the likelihood that a computer-generated limit set is a strange attractor have not yet been developed.

Having said that, I shall pretend that some of our cubic maps do illustrate strange attractors. How can those maps be studied further? One way is to introduce another variable δ ($0 < \delta \leq 1$). Letting $S' = F(S, \alpha)$ and $\alpha' = G(S, \alpha)$ denote the defining equations of the map (cf. Eq. 11b), we write a new set of equations as follows:

$$\begin{aligned} S' &= (1-\delta)S + \delta F(S, \alpha) \\ \alpha' &= (1-\delta)\alpha + \delta G(S, \alpha). \end{aligned} \tag{12}$$

Note that $\delta = 1$ corresponds to the original map. (If $\delta = 0$, Eq. 12 reduces to the identity transformation.) So long as δ lies in the given range, the first-order fixed points are independent of this parameter. The original system may have a nonattractive fixed point; it cannot, of course, be found by iteration. If, however, the fixed point can be made attractive by decreasing δ (from unity), then iteration can be used, thus avoiding some messy algebra. In fact, a sufficient decrease in δ will—in almost all cases—decrease the absolute value of both eigenvalues of the Jacobian matrix of Eq. 12 to less than unity at the fixed point, which is precisely the criterion for the attractive



EFFECT OF δ ON THE LIMIT SET OF T_A

Fig. 9. Our two-dimensional cubic maps can be generalized by introducing the parameter δ as described in the text. Shown here is the effect of varying this parameter on the messy limit set of T_A (see Fig. 8). As δ is decreased from unity, the limit points at first coalesce into seven distinct bunches, forming what we call a pseudo-period. (a) Then at $\delta \approx 0.9930$, the infinite limit set becomes periodic (and hence finite), with an order of 7. (b) This configuration persists over a range of δ values, although the coordinates of the limit points vary. (c) Then at $\delta \approx 0.9770$, the periodic limit set changes into a closed curve. (d) As δ is decreased further, the curve becomes smaller and smaller. Finally, at $\delta \approx 0.9180$, the curve collapses to a single point, the nonattractive fixed point of the original transformation ($\delta = 1$).

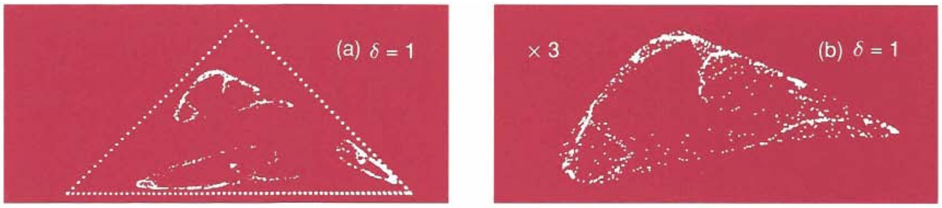
character of such a point. This is the fact that motivated the introduction of δ, but the effect of its variation turned out to be much more interesting than we expected. Decreasing δ may cause a remarkable change in the appearance of a messy limit set (Fig. 9). Points may start to cohere, forming a pattern of disjoint arcs. Further decrease of δ may lead to a periodic limit set of finite order, which persists over a range of δ values. As δ approaches the value at which the limit set collapses to the fixed point, the set may metamorphose into a closed curve (at least something that looks like a curve) that shrinks continuously with δ. This behavior is typical; even more complex changes have been observed in some cases (Fig. 10).

Another way to study cubic maps with messes as their limit sets is to vary the coefficients. This is done just as it was for the quadratic maps, but the results are far more dramatic. Figure 11 shows a few examples of the fascinating behavior that has been observed. Here the coefficients constitute a twenty-parameter set, so exploration of all possibilities is not feasible; the usual practice is to vary the coefficients of one or two terms at a time. Much numerical work of that type was done at the Laboratory in 1984 and 1985 on a Cray computer, and many new strange attractors turned up. The aim of this work is to find some "structural" (geometric or algebraic) principle underlying the relatively bizarre phenomena our computer screens reveal.

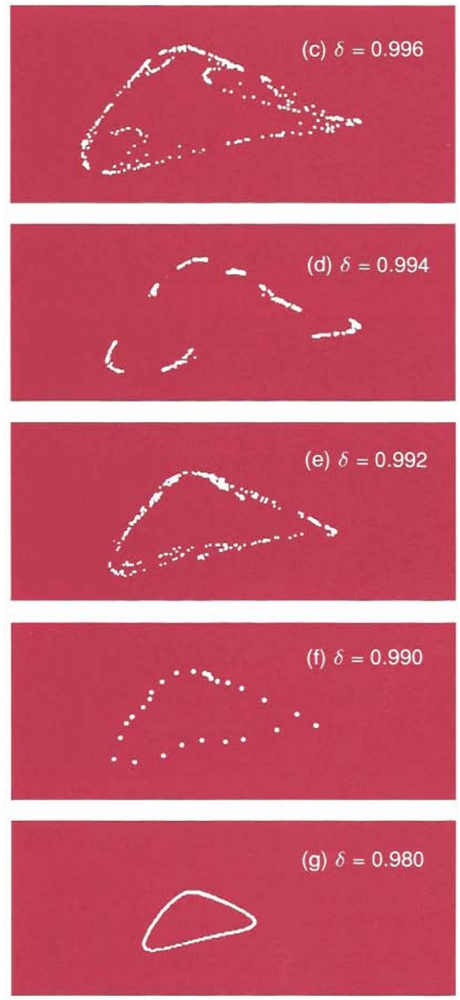
One-Dimensional Maps and Universality

The first part of this section is a historical note on the origins of a 1973 paper by Metropolis, Stein, and Stein. The paper dealt with a certain universal structure and hierarchy of the periodic limit sets that can arise in the iteration of one-dimensional maps; it has been cited by Mitchell Feigenbaum as a source of inspiration for his later work on the universal nature of the approach to chaos by "period doubling."

The origins of our paper lie in the work discussed above by Stan and me on cubic maps. We had found fifteen or sixteen that had the property of transforming a pair of sides of the S, α reference triangle into each other. It is clear that the "square" of such a map (the second iterate) transforms one side of the triangle into itself, and the map is therefore one-dimensional. We rewrote some of these as maps defined on the unit interval and iterated them on MANIAC II. In every case we obtained a periodic limit



$T: x_1' = x_2^3 + 3x_1x_2^2 + 3x_2x_1^2 + 3x_2x_3^2 + 3x_3x_2^2,\ x_2' = 3x_1x_3^2 + 3x_3x_1^2 + 6x_1x_2x_3,\ x_3' = x_1^3 + x_3^3$



set of high order (1500 or thereabout). We had reasons for thinking that these results were spurious, caused by the limited precision of the machine, and that what we were seeing were artifacts. Indeed, when we iterated the two simpler maps

$$x' = 4x(1-x), \quad 0 \le x \le 1 \tag{13a}$$

and

$$x' = \sin \pi x, \quad 0 \le x \le 1, \tag{13b}$$

we also found high-order periods. For these maps, however, it was easy to prove that no such limit sets could exist, so our suspicions were confirmed. A year or two later the IBM 7030 ("Stretch") became available. With its larger word size, it failed to reproduce our impossible periods.

In 1970 Nick Metropolis and Myron Stein joined me in an attempt to find out what was really going on in all these one-dimensional examples. Of course, we could not resist generalizing the problem slightly by introducing a parameter λ, essentially the height of the map in a plot of x' versus x. For instance, instead of Eqs. 13a and 13b we wrote

$$x' = \lambda x(1-x), \quad 0 \le x \le 1 \text{ and } 3 < \lambda < 4 \tag{14a}$$

and

$$x' = \lambda \sin \pi x, \quad 0 \le x \le 1 \text{ and } \approx 0.71 < \lambda < 1. \tag{14b}$$

The restrictions on λ insure that the iterates of the maps lie within the specified x interval and that the nonzero first-order fixed points of the maps are nonattractive. (Equation 14a, the "parameterized parabola," is well known in ecology as the logistic equation. It is a transform of a quadratic map studied in the early sixties by the Finnish mathematician P. Myrberg. Had we been aware of his study, considerable time would have been saved.)

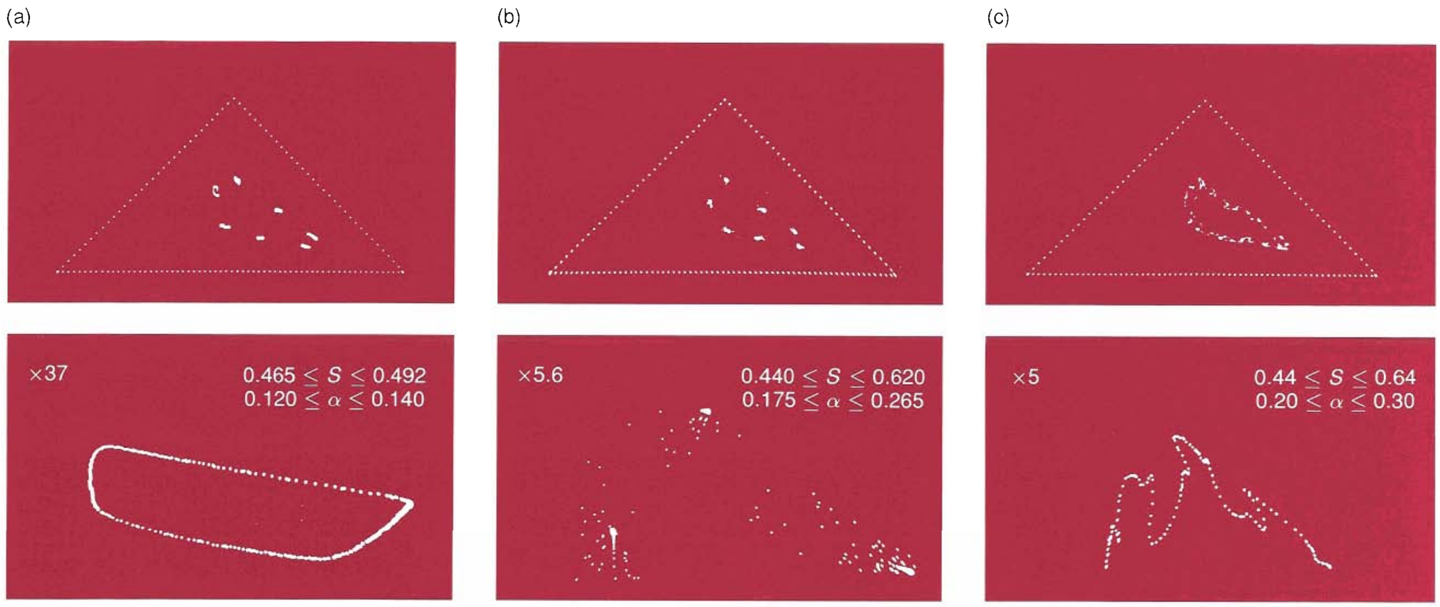
Equations 14a and 14b are examples of maps of the general form

$$T_\lambda(x) : x' = \lambda f(x),$$

where $f(x)$ is defined on the interval [0,1] and has a single maximum (at which $dx'/dx = 0$). For simplicity we placed the maximum at $x = \frac{1}{2}$ and at first restricted ourselves to functions symmetric about that point. This restriction does not affect the results presented in the "MSS" paper (a name due to Derrida, Gervois, and Pomeau). We also required $f(x)$ to be strictly concave; relaxing this requirement can have drastic effects, as we learned later.

ANOTHER EXAMPLE OF THE EFFECT OF δ ON A MESSY LIMIT SET

Fig. 10. An even more striking example of the effect of varying δ on a messy limit set. (a) The limit set for the original two-dimensional cubic map (δ = 1) consists of three separate pieces. Photographs (c) through (g) focus on the changes that occur in the piece shown in greater detail in (b); similar changes occur in the other two pieces. As δ is decreased monotonically from unity, the limit points (c) consolidate, (d) form a set of disjoint arcs, (e) disperse, (f) collapse to a periodic limit set of order 26, and (g) form a closed curve that eventually collapses to a single point.



$$\begin{aligned} T_A(\text{modified}):\ x_1' &= x_3^3 + 3x_1x_3^2 + 3x_2x_3^2 \\ &\quad + 3x_3x_2^2 + 6x_1x_2x_3 \\ x_2' &= x_1^3 + 0.91x_2^3 + 3x_3x_1^2 \\ x_3' &= 3x_1x_2^2 + 3x_2x_1^2 + 0.09x_2^3 \end{aligned}$$

$$\begin{aligned} T_A(\text{modified}):\ x_1' &= x_3^3 + 3x_1x_3^2 + 3x_2x_3^2 \\ &\quad + 3x_3x_2^2 + 6x_1x_2x_3 \\ x_2' &= x_1^3 + 0.97x_2^3 + 3x_3x_1^2 \\ x_3' &= 3x_1x_2^2 + 3x_2x_1^2 + 0.03x_2^3 \end{aligned}$$

$$\begin{aligned} T_A(\text{modified}):\ x_1' &= x_3^3 + 2.88x_1x_3^2 + 3x_2x_3^2 \\ &\quad + 3x_3x_2^2 + 6x_1x_2x_3 \\ x_2' &= x_1^3 + x_2^3 + 3x_3x_1^2 + 0.12x_1x_3^2 \\ x_3' &= 3x_1x_2^2 + 3x_2x_1^2 \end{aligned}$$

EFFECT OF COEFFICIENTS ON THE LIMIT SET OF T_A

Fig. 11. Our two-dimensional cubic maps can also be generalized by varying the coefficients. In the examples above the transformation T_A was modified by varying only two coefficients. The photographs show the dramatic effect of such modifications on the messy limit set of T_A (Fig. 8). The modification given in (a) changes the mess into a seven-member set of closed curves, one of which is shown in detail. The very similar modification given in (b) changes the mess into a pseudo- period of order 7, that is, into seven distinct bunches of points, three of which are shown in detail. The modification given in (c) results in a remarkably different but still messy limit set.

In addition to the parabola and the sine, we also studied two other functions satisfying the conditions given above. One, a sixth-degree polynomial, was the transform to the unit interval of one of the one-dimensional cubic maps mentioned previously; the other was a trapezoid (in the x',x plane).

For all four maps we calculated the periodic limit sets of order k that begin and end with $x = \frac{1}{2}$. These correspond to λ values that are solutions of

$$T_\lambda^{(k)}\left(\frac{1}{2}\right) = \frac{1}{2}$$

and are necessarily attractive because of the condition that $dx'/dx|_{x=\frac{1}{2}} = 0$. (This condition guarantees what is referred to as superstability.) To characterize the limit sets in a function-independent way, we used the minimum distinguishing information, namely, the positions of the successive iterates relative to $x = \frac{1}{2}$. For this purpose we employed the letters R and L ("right" and "left"). For example, when $k = 5$, all our maps have three distinct periodic limit sets of order 5, each associated with a different value of λ. Naturally, for different functions the λ values are different, as are the actual values of the iterates, but the R, L (or MSS) patterns are identical. The three patterns for $k = 5$, in order of increasing λ, are $\frac{1}{2} \to R \to L \to R \to R \to \frac{1}{2}$, $\frac{1}{2} \to R \to L \to L \to R \to \frac{1}{2}$, and $\frac{1}{2} \to R \to L \to L \to L \to \frac{1}{2}$. Omitting the initial and final $\frac{1}{2}$'s, we may write these patterns in simplified form as RLR^2, RL^2R, and RL^3.

The identity of the MSS patterns and their ordering on λ was found to hold among all of our four functions for all values of k such that $2 \leq k \leq 15$. We immediately noted the phenomenon that Feigenbaum later called period doubling. As an example, consider the period of order 2, the pattern of which is R. The patterns of its first two doublings are RLR ($k = 4$) and RLR^3LR ($k = 8$). A simple rule relates the pattern P of a given period and that of its doubling: if P contains an odd (even) number of R's, the pattern of its doubling is PLP (PRP). Note that P must be an MSS pattern; that is, it must begin and end at the x value for which x' is maximum. (Obviously, not every R, L succession is such a pattern.)

Period doublings are, of course, ordered on increasing λ. The λ values corresponding to two successive doublings, λ_1 and λ_2, are "contiguous" in the sense that no λ between λ_1 and λ_2 corresponds to a periodic limit set beginning at $\frac{1}{2}$.

Our initial work indicated that a large class of maps generates the same sequence of patterns ordered on increasing λ. Later experiments on some fifty additional maps confirmed this conclusion. It is still not known exactly, however, how this "large class" (almost certainly infinite) should be defined.

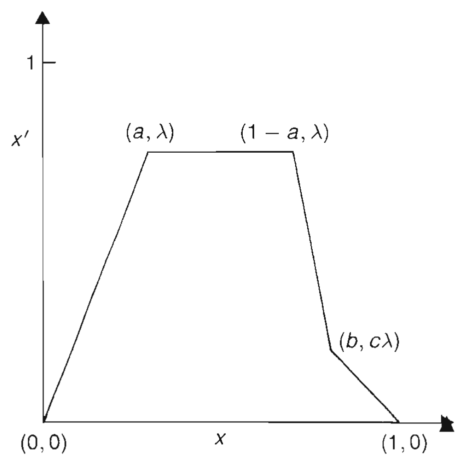
One of the most interesting results presented in the MSS paper is an algorithm for generating the MSS sequence. No iterations are needed, and no functions are explicitly specified. The algorithm is purely logical; given a limiting value $k_{\max}$ for the period order, it produces all MSS patterns with $k \leq k_{\max}$ in the canonical ordering (that is, on increasing λ). An independent proof of this algorithm is given for trapezoidal maps in Louck and Metropolis 1986. Others have found new algorithms for generating the MSS sequence, but, in my opinion, none of these are substantially simpler than ours.

Since the publication of these results, many mathematicians and physicists have studied one-dimensional maps, but much more work has been done on Feigenbaum's "quantitative" universality than on the "structural" universality represented by the MSS sequence. A few years ago Bill Beyer, Dan Mauldin (of North Texas State University), and I initiated new attacks on some of the problems suggested by MSS. We also considered a few new questions. One of these has to do with maps that exhibit a multiple appearance of some MSS patterns. If a map is strictly concave, it is our conjecture that each pattern occurs for just one value of λ. We found that something else can happen otherwise. Consider the "indented trapezoid" map shown in Fig. 12, which is not strictly concave. For certain ranges of the parameters b and c, the same MSS pattern corresponds to three different λ values. (This phenomenon implies that Feigenbaum's quantitative universality, which hinges on the occurrence of period doublings at unique λ values, is not applicable to certain maps and hence is less than truly universal.)

Our multiplicity, as we called it, is more than an interesting mathematical fact. It has helped in understanding the latest results of an extensive study of the Belousov-Zhabotinskii reaction by H. L. Swinney and his collaborators. (The B-Z reaction, the oxidation of malonic acid by an acidic bromate solution in the presence of a cerous ion catalyst, is an oscillating chemical system, that is, a system in which the concentrations of the chemical species do not vary monotonically with time but instead oscillate, sometimes chaotically, sometimes periodically.) In 1982 Simoyi, Wolf, and Swinney had identified certain members of the MSS sequence in the periodic concentration variations of the bromide ion, one of some thirty chemical entities involved in the reaction. In addition they found that the MSS patterns observed were ordered on a parameter τ (the residence time of the reactants in the reaction vessel, which is inversely proportional to their rate of flow through the vessel) in exactly the same manner as the patterns in the MSS sequence are ordered on λ. Several years later

THE "INDENTED TRAPEZOID" MAP

Fig. 12. Because it is not strictly concave, the "indented trapezoid" map exhibits "multiplicity"; that is, it does not exhibit a one-to-one correspondence between MSS patterns (see text) and λ values. In particular, for certain ranges of the parameters b and c, some of the patterns correspond to three values of λ.



$$\frac{1}{2} < b < 1$$

$$a + b \neq 1$$

$$c > \frac{1-b}{a}, \quad \frac{1}{2} < a + b < 1$$

$$0 < c < \frac{1-b}{a}, \quad 1 < a + b < \frac{3}{2}$$

$$\begin{aligned} T : x' &= \frac{\lambda}{a} x, \quad 0 \leq x \leq a \\ &= \lambda, \quad a \leq x \leq (1-a) \\ &= \lambda \frac{(c-1)x + c(a-1)}{a+b-1}, \\ &\quad (1-a) \leq x \leq b \\ &= c\lambda \frac{1-x}{1-b}, \quad a \leq x \leq 1 \end{aligned}$$

Coffman, McCormick, and Swinney made further measurements on the system, this time controlling the flow rate much more precisely. Again they found members of the MSS sequence, but some of the patterns occurred for three values of τ. At that time they knew nothing of our recent work on the indented trapezoid and suspected that their strange results were due to some systematic error. How they came to learn of multiplicity was a matter of pure chance. Swinney was visiting North Texas State (where Mauldin teaches mathematics) to give a talk. His hosts, looking for some way to amuse him between lunch and the colloquium, brought him to Mauldin's office. To pass the time, Dan started to discuss our discovery. Swinney immediately realized that what he and his colleagues had seen was not, after all, an artifact. They went on to identify the analogue of the indentation parameter c as trace impurities in one of the reactants. It is certainly gratifying when some purely mathematical construct helps to explain physical reality.

Number Theory

Stan Ulam's name seems to have disappeared from these pages; it is time to bring it back, if only briefly. Stan was not a number theorist, but he knew many number-theoretical facts, some of them quite recondite. As all who knew him will remember, it was Stan's particular pleasure to pose difficult, though simply stated, questions in many branches of mathematics. Number theory is a field particularly vulnerable to the "Ulam treatment," and Stan proposed more than his share of hard questions; not being a professional in the field, he was under no obligation to answer them.

Stan was very much interested in "sieve" methods—the sieve of Eratosthenes to generate the primes is the most famous—but from an experimental rather than an analytic viewpoint. He was always trying to invent new sieves that would generate sequences of numbers that were in some sense prime-like. His greatest success was the "lucky number" sieve (the name is derived from a story in Josephus's *History of the Jewish War*). In Eratosthenes's sieve one crosses out 1 from a list of the integers and then, keeping 2 (the first prime), crosses out all of its other multiples. The first survivor after 2 is 3, so next one crosses out all of its higher multiples, and so on. In the lucky number sieve one first crosses out every second number, that is, *all* the evens; in fact, one throws them out of the list, which is consequently collapsed. The first survivor after 1 is 3, so, again starting from the beginning, one throws out every third number, collapsing the list further. The next survivor is 7, so one then throws out every seventh number, and so on. The first ten lucky numbers are 1, 3, 7, 9, 13, 15, 21, 25, 31, and 33. All lucky numbers less than 3,750,000 were known by the early sixties. (Compared to the sieve for the primes, the lucky number sieve is rather slow.) Perhaps progress has been made, but I doubt that the range has been increased by a factor of 100 to match our current knowledge of the primes.

Although the lucky numbers are clearly not a multiplicative basis for the integers, they do have some prime-like properties. For example, their asymptotic distribution is, to first order, the same as that of the primes (Hawkins and Briggs). The luckies are, however, somewhat sparser than the primes, as, if I am not mistaken, Stan predicted. (Expressions for p_n, the nth prime, and ℓ_n, the nth lucky number are

$$p_n = n \ln n + n \ln(\ln n) + \text{higher order terms}$$

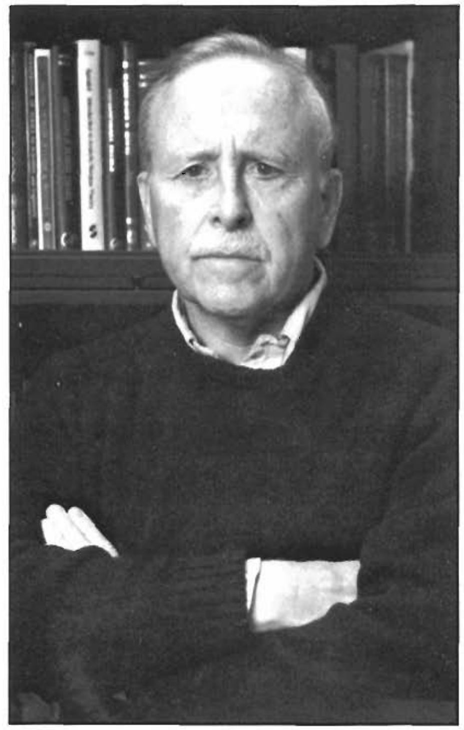
and $$\ell_n = n \ln n + \frac{1}{2} n \left(\ln(\ln n)\right)^2 + \text{higher order terms.}$$

Of course these expressions make sense only for large n. Nevertheless, if we (recklessly) disregard the higher order terms, they imply that $\ell_n > p_n$ for $n > 1619$. In fact, however, we find that $\ell_n > p_n$ for $11 \leq n \leq 3,750,000$.) The distribution of the lucky numbers is similar to that of the primes in another respect: there seem to be an infinite number of lucky "twins," that is, luckies whose difference is 2. The evidence for this is far from overwhelming because the lucky sieve is hard to implement on a computer.

What I learned from Stan's ventures into number theory was that amateurs can make useful contributions to the field. That moved me to launch an attack on my favorite classical problem, the Goldbach conjecture. This is the statement, made by Christian Goldbach in a letter to his friend Euler, that every even integer equal to or greater than 6 is the sum of two odd prime numbers in at least one way. It remains unproven to this day, although very few mathematicians have doubts about its truth. Curiously, the analogous problem for odd integers, namely, that from some point on, each is the sum of three odd primes, was proved by Vinogradov in 1937. His original proof is long and difficult; it may have been at least a decade before its correctness was generally admitted. As for the Goldbach conjecture, the best result to date is that all sufficiently large even integers can be expressed as the sum of a prime and an integer that has at most two prime factors. This result, due to J.-R. Chen, is considered to be the greatest triumph ever achieved by sieve methods. That the Goldbach "property" is true for lucky numbers was conjectured by Stan, and work by Myron Stein and me gives some support. Stan's conjecture should not be too surprising in view of a 1970 study by Everett and me, which shows that almost all sequences with overall prime-like distributions have both the twin property and the Goldbach property. (Here "almost all" is to be understood in a measure-theoretic sense.)

In the mid sixties Myron Stein and I decided to look at the Goldbach problem numerically. We started by examining the so-called Goldbach curve, that is, the plot versus the even numbers of the total number of ways of expressing each as the sum of two primes. The curve is rather bumpy, usually peaking locally at multiples of 6 (as explained in the introduction to Stein and Stein 1964). Clearly many more primes exist than are necessary to constitute an additive 2-basis for the even numbers. This motivated us to look for sparse subsets of the primes possessing that property ("S" bases). We found a good algorithm (the S algorithm) for producing such subsets; each is completely determined by the choice of a smallest prime p_0. Our S bases cover almost all the evens from $2p_0$ to 10,000,000, leaving uncovered only a few low evens at the start. The sparseness achieved is striking; with one exception the S bases consist of less than 1.6 percent of the primes less than 10,000,000. The exception is the basis beginning with 7, which contains roughly twice as many primes as any other (a fact still unexplained). Our conclusion from this work is that the Goldbach property does not critically involve the famous prime property of being a multiplicative basis for the integers.

In concluding I must mention that the above investigation of the Goldbach problem moved the number theorist Daniel Shanks to convey on those involved the title "Los Alamos School of Experimental Number Theory." As to this new institution, there is no doubt that Stan Ulam was the founder. ■



Paul R. Stein has been a staff member at the Laboratory since 1950, working on problems that range from mathematical biology to nonlinear transformations and experimental number theory.

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