CATASTROPHE THEORY IN SCIENTIFIC RESEARCH

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Thom's theorem has been described, in some of the more unrestrained accounts, as defining all discontinuous changes that can ever occur in spacetime. This has obscured the ways in which the techniques behind the theorem improve the cutting edge of the most traditional calculation methods of science. The same techniques lead, as this article illustrates from the authors' research, to analyses of phenomena not on the famous list of 'seven elementary catastrophes' but arising naturally in fields as diverse as crystal phase transitions, nonlinear elasticity, and population distribution.

Much of the controversy surrounding catastrophe theory stems from the claim that it provides a 'universal set of models for discontinuous phenomena'. This claim needs severe qualifications to be tenable, and has appeared doubtfully useful to the scientist dealing with particular phenomena. The resulting debate, often revolving around whether "That is a cusp catastrophe!!" represents information or not, has somewhat obscured the ways in which the cluster of results known as Thom's Theorem can refine the usual computational equipment of the sciences. (We discuss and illustrate some of these ways below.) Moreover, the 'physical examples' offered by mathematicians have often been 19th century physics, as that is all the physics in the usual mathematical education. Since significant applications of new mathematics comes only from its use on current problems, its utility appears only slowly unless (like the Dirac δ-function) it is invented by a nonmathematician. But since catastrophe theory involves a sharpening of some very traditional tools, it should be useful wherever these are used.

A physical audience often greets catastrophe theory with essentially the reply,

"This is just Taylor series.
We know about Taylor series."

Yes and no; catastrophe theory and the surrounding mathematics consist fairly exactly of what mathematicians have learned about Taylor expansions in the last decade or so.

First, mathematical attention has shifted from (infinite) Taylor series to (finite) Taylor expansions to order k. This is appropriate to their practical uses, which usually involve the calculation of a finite number of terms. Such calculations are often prefaced by the hypothesis that the function, f, involved is analytic. This hypothesis depends on strong assumptions: that the infinite Taylor series of f converges, and that the result coincides with f. Indeed, any power series, convergent or pathological, can occur as a Taylor series, while even a convergent series may not be a good description of f. (The function $f(x) = \exp(-1/x^2)$, for $x \neq 0$, $f(o) = 0$, is infinitely differentiable and has an absolute minimum at 0. Its Taylor series at 0 vanishes identically.) But even these strong assumptions are not sufficient (Box 1) to justify even qualitatively the use of only a finite number of terms.

Nor in fact are they necessary.

Box 2 illustrates in a familiar context the idea of 'determinacy': for real functions of one real variable, the 'local shape' is always fixed by the first nonconstant term in the Taylor expansion. For functions of two or more variables this is false in general, as in Box 1. But for 'almost every' smooth function $f(x_1,\ldots,x_n)$, in a strong sense, the local form of f is determined up to a smooth change of variables by its Taylor expansion $j^k f$ at 0 to order k, for some finite k; f is *k-determinate* at 0.

The determinacy of a particular f may be settled by appeal to a theorem of Mather, whose use requires only elementary linear algebra. A detailed account with worked examples, and without the language of 'ideals in the ring of germs at 0 of C^∞ functions' necessary for a proof, may be found in [1].

The results may be unexpected;

$$f(x,y) = x^3 + y^3 + r_4(x,y)$$

is 3-determinate and reducible to the

Suppose

$$f(x,y) = x^2e^xy = x^2y + x^3y + \frac{x^4}{2!}y + \ldots$$

Then the equation

$$f(x,y) = 0$$

has exactly the x and y axes as solutions (Fig. 1a). But if

$$g(x,y) = x^2e^xy + \frac{y^{100}}{100!},\ h(x,y) = x^2e^xy + \frac{y^{101}}{101!},$$

the equations

$$g(x,y) = 0, \quad h(x,y) = 0$$

have respectively no solutions for $y > 0$ and none for $y \neq 0$ (Fig. 1b,1c). All of f, g and h are analytic, and agree to order 100: we could as easily have made it 10^{100}. No number of terms agreeing with f will guarantee that an analytic function looks like f and not g or h.

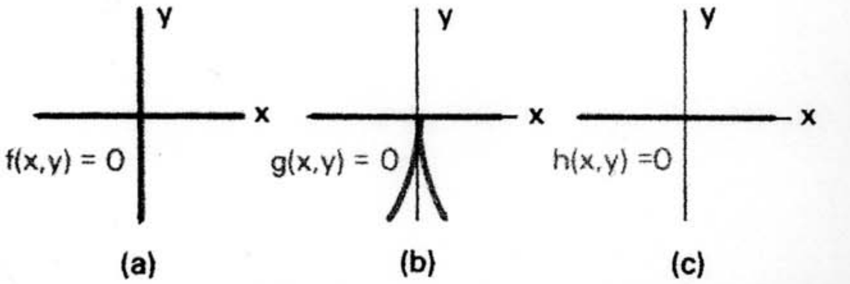

FIGURE 1. The graphs of three quite different functions whose Taylor series are identical to 100 terms.

BOX 1

local form $u^3 + v^3$, as one might guess, but

$$g(x,y) = (x+y)^2 + x^3 + y^3$$

is only 4-determinate. Any 5th-order addition can be removed locally by a smooth change of coordinates, but (unlike g) the function $g(x,y) + 4y^4$ has no negative values for (x,y) near the origin.

These determinacy rules establish just how far one need go in a Taylor expansion when seeking certain kinds of information. They are of practical use in dealing with particular 'real world' functions, and should be included routinely in Applied Mathematics courses. They are also completely algorithmic (although of course laborious in complicated cases) and could be included in any standard software package that handles symbolic differentiation.

UNFOLDINGS

Whenever a function $f(x_1,\ldots,x_n)$ is k-determinate at 0, it has a finite-dimensional *universal unfolding*, which describes the effect of any small perturbation whatever on its geometry. For

$$f(x,y) = x^2 + y^2,$$

no small perturbation changes the property of having a simple minimum. When f is locally reducible by the determinacy rules to

$$x^2 + y^4,$$

the effects of all possible small perturbations are described by the *cusp catastrophe*, here taking the form

$$x^2 + y^4 + ay^2 + by,$$

whose geometry is analyzed in [2] and elsewhere. This example shows the way in which a universal unfolding not only classifies the nearby functions but also gives the geometry of the way the unfoldings surround f and depend on the 'unfolding variables' a and b. This finding has applications to civil engineering (where it yields exact values for exponents known as 'imperfection sensitivities'), to wave propagation (where it yields relations on intensities at caustics, needed, for example, for calculation of sonar transmission losses), and so forth. The theorems establishing the universality of these families of perturbations are deep, capturing the effect of *all* small perturbations of the function near the point of interest, not merely 'almost all'. But the calculations required in particular cases are a simple extension of those for determinacy. They are described in the same elementary (though cumbersome) language in [1].

THE SEVEN ELEMENTARY CATASTROPHES

One often reads that the seven universal unfolding geometries with up to four unfolding variables provide a universal set of models. This is true as stated and proved in the mathematical treatments of the theory[1], but false as expressed in many popularized accounts. First, not all discontinuous processes can be reduced to the bifurcation of a single real-valued function, such as phase intensity, entropy or a Liapunor function. Thus the theory may not apply. Secondly, when it does apply, the theory says only that these models cover *almost all* bifurcations, in a topological and partly measured theoretic sense. The precise statement is intuitive only to a topologist, but its strengths and limitations are displayed by the analogous way that *almost all* curves in (x,y,z)-space fail to meet the x-axis, while those that do may easily be perturbed off it. Indeed, the result is obtained from exactly this kind of geometric fact. (For a formal treatment see [3]; for a pictorial account of the way one leads to the other see [4].) But what if the situation has an essential symmetry? Curves symmetric under

$$(x,y,z) \mapsto (x,y,-z)$$

are restricted to the (x,y) plane, and it is far from typical that they should miss the x-axis. *Subject to the symmetry condition*, they can do so stably.

In strict analogy, the family

$$f_a(x) = x^4 + ax^2$$

provides a universal unfolding of x^4 within the restricted class of even functions (Figure 3). Subject to this symmetry condition, it can occur

If a function $f(x)$ has the form

$$f(x) = c + x + r_2(x),$$

where $r_2(x)$ has zero slope at 0, f is increasing near 0 (Fig. 2a). If

$$f(x) = c + x^2 + r_3(x)$$

where the first and second derivatives of r_3 vanish at 0, f has a minimum at 0 (Fig. 2b). And so on. Simple analysis shows that for any

$$f(x) = c + x^n + r_{n+1}(x)$$

with the first n derivatives of r_{n+1} vanishing at 0, there is a smooth change of coordinates $y(x)$ near 0 giving f the form $c + y^n$ *exactly*. The degree of 'smoothness' of the change from x to y depends on how many times f is continuously differentiable after the n^{th} derivative, but the removal of the 'Taylor tail,' r_{n+1}, does not require that f be analytic. The analogous recent results for $f(x_1,...,x_n)$ are discussed in the main text.

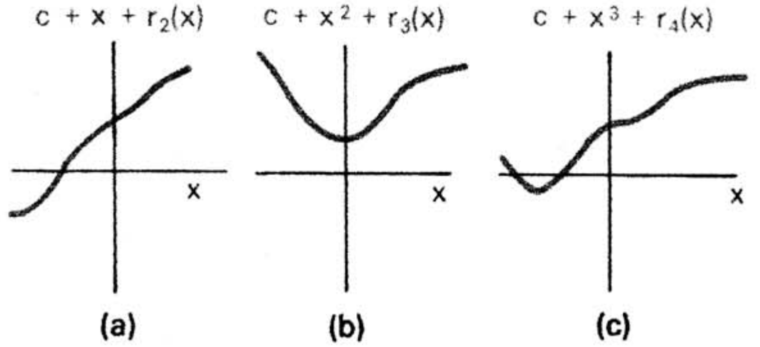

FIGURE 2. Graphs 'determined' around by finite Taylor expansions.

BOX 2

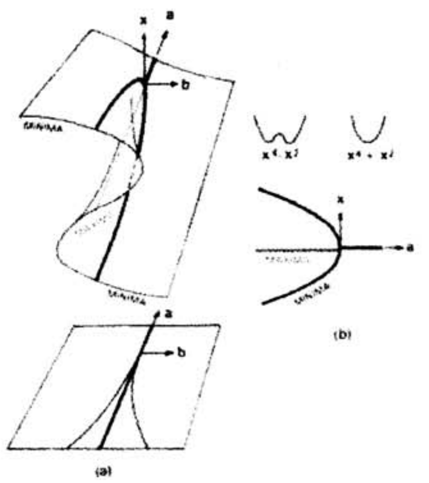

FIGURE 3a. 'Universal' bifurcation diagrams around x^4.

FIGURE 3b. Bifurcation diagram around x^4, universal for perturbations that maintain the symmetry $x \mapsto -x$. (Note that x^4-x^2 has this symmetry, though its minima individually have not.)

Almost all 2-parameter families $f_{(a,b)}(x,y,z)$ of functions invariant under a 90° turn about the z-axis can be reduced locally to one of the following forms by a smooth change of coordinates.

$\pm(x^2 + y^2) + z^3 + az$

$\pm(x^2 + y^2) \pm z^4 + az^2 + bz$

$(x^4 - 6x^2y^2 + y^4) + \alpha(x^2 + y^2)^2 \pm z^2 + a(x^2 + y^2)$, some $\alpha \neq \pm 1$.

$\pm[x^2y^2 + \alpha(x^2 + y^2)^2] + a(x^2 + y^2)^2 + b(x^2 + y^2)$, some $\alpha \neq 0$.

$\pm[(x^2 + y^2)z \pm z^3 + \alpha x^2y^2] + az^2 + bz$, some $\alpha \neq 0$.

(Each of the last three is an infinite family of possibilities, parameterized by the number α. For the way in which such infinite families arise, see [4].

Any family not so reducible can be made so by an arbitrarily small perturbation. This does not mean that it is physically impossible, but suggests that a physical justification for its specialness is called for if it is used for exact calculations.

Analogous lists apply for the other 31 crystallographic point groups.

BOX 3

stably, though in the general setting a one-parameter family of functions cannot stably meet functions locally expressible as x^4. (And the 'typical' one-parameter family is stable and does avoid such points; for a detailed pictorial explanation, see [4].

Other types of restriction can stablize behaviors that in the general space of functions are 'untypical' and unstable, but symmetries are probably the most important types in physics. Within any restricted class the general problem of identifying the typical phenomena is again of interest. For real-valued functions invariant under finite or compact groups, analogues to the key theorems of the unsymmetric case have been proved. We are applying these analogues to the classification of the generic bifurcations of real-valued functions $f(x,y,z)$, subject to symmetry under each of the 32 crystallographic point groups (Box 3). These analogues described the typical geometries of changes in type of thermodynamic potentials invariant under each group, under external variation of such quantities as temperature and pressure. (The physics of the corresponding phase transitions, of course, depends also on an analysis of such factors as the effects of fluctuations.) The analogues also describe canonical local changes in type for the branches of a dispersion relation, yielding information about the singularity structure of the vibrational or electronic spectrum of crystals with the specified symmetry.

In these bifurcations the symmetry involved is retained by the set of extrema, as in Figure 3b, though not by its members. However, if symmetry is imposed by design and not by nature, the designer is attempting a highly special, 'nongeneric' system. (S)he must consider asymmetric perturbations of what is achieved. For example, the symmetries of the buckling plate described by the von Kármán equation force bifurcation at a double eigenvalue to be governed by one of the eight-dimensional Double Cusp catastrophes. (These are common for just this kind of reason.) We are working with Robert Magnus of Battelle-Geneva on a full description of this buckling structure. Our work involves a fruitful synthesis of the infinite-dimensional techniques of the functional analysts' version of bifurcation theory, which has traditionally restricted attention to one-parameter families of operators, with Thom's concept of the k-parameter *universal* unfolding of a function $f(x_1,...,x_n)$, which was first defined in finite dimensions.

Dr. E. Ascher (left) joined Battelle-Geneva in 1955 after receiving his Ph.D. from the University in Lausanne. His work includes studies in mathematical crystallography, the phenomenological theory of phase transitions and the relation between symmetries and properties of physical systems. He now is using catastrophe theory for the understanding of symmetry breaking. He also is studying the problems of mathematical modelling in the social sciences (see *Research Futures*, 1974/3) and works with Jean Piaget on these aspects in relation to epistemology. He was president of the Swiss Crystallographic Society (1973-1975) and now is a member of the senate of the Swiss Academy of Sciences.

Dr. Tim Poston received his Ph.D. in Mathematics from the University of Warwick (England) in 1972 and taught in Rio de Janeiro, Rochester (NY) and Oporto before joining Battelle-Geneva in February 1975. He has worked on the coordinate-free formulation of finite difference equations, the geometry of crystal spectrum computations, and catastrophe theory. His publications include a volume of Springer Lecture Notes in Mathematics (with A.E.R. Woodcock) on the geometry of the elementary catastrophes, and a geometry and relativity textbook (with C.T.J. Dodson) to appear in Spring 1977, besides the notes on catastrophe theory discussed in this article.

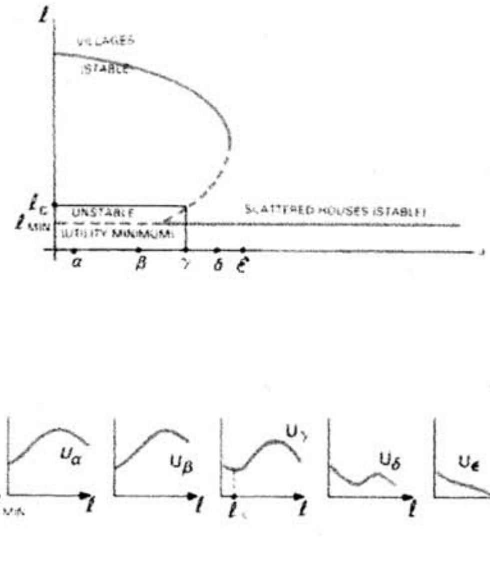

FIGURE 4. Local maxima (solid) and minima (dotted) of total utility $U_a(\ell)$ as a function of correlation distance ℓ, for different values of an agricultural parameter a. Graphs of representative U_a's are also shown.
Weakening the hypotheses of the model adds "catastrophes" rather than removes them.

CONSTRAINT CATASTROPHES

Recent work with Professor Colin Renfrew of Southampton University has shown that the simplest reasonable assumptions on the utility functions involved generate a model which predicts discontinuous changes of population distribution in early agricultural communities (Figure 4). A detailed report is in preparation, but a point of independent interest is the transition between U_β and U_γ. Since ℓ is constrainted to exceed a value ℓ_{min} (representing the most evenly scattered population), a local minimum for U_β at ℓ_{min} can become for U_γ a maximum at ℓ_{min} and a minimum at ℓ_c. This phenomenon does not appear on Thom's list, since Thom's hypotheses involve *interior* bifurcations only, but in the presence of positivity constraints (such as are universal in the social sciences) it can occur stably. *Only* this and Thom's fold catastrophe, in fact, can occur stably in a maximization problem in n dimensions for a system with one varying external parameter if no special conditions (linearity, symmetry, etc.) are imposed. It is the simplest of the *constraint catastrophes*. These are distinct from Thom's magnificent seven, but can be classified, analyzed and used computationally by similar techniques; the classification becomes technically infinite with four external parameters, rather than six as in Thom's Theorem.

CONCLUDING REMARKS

Catastrophe theory, like the calculus of which it is a part, will in the course of time become part of the routine mathematics of science. It is easy to misuse its theorems, like those of statistics, if their hypotheses are not understood. (We might cite the widespread use of computer-packaged regression analysis with data that is not *a priori* even unimodally, let alone normally, distributed.) Suffice it to say that all mathematics is something like a chisel. When it is used as a hammer, the results are usually remarkable and occasionally fatal.

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