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Experimental Mathematics

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1. Experimental mathematics is nothing new; in fact, it predates mathematics itself. In ancient societies people gradually developed, by experiments, systems of numbers and rules for computing with them long before they codified these into formal definitions, theorems and proofs. Something similar probably happened in geometry and, to a certain extent, later, in other branches of mathematics.

Note also that many children showing a keen interest in mathematics, including those who grow up to become eminent mathematicians, explore elementary mathematics in an experimental fashion, say, examining numbers for properties raising their curiosity.

2. In this note we make some remarks on experimental mathematics, speculate on its future and describe a mathematical experiment. But our main purpose is to suggest that experimental mathematics organizes into a science of its own, complete with its journals, conferences, courses of instruction, etc.

3. One way of looking at mathematics is considering it a superposition of two sciences. The first studies certain abstract objects: numbers, functions, etc. The second is the axiomatic method. Part of the first science could have been studied experimentally as is done in elementary school arithmetic. In fact, one can imagine a civilization in which some of the first science is developed experimentally to a high level without use of the second or, what seems easier to imagine, the first science includes both theories arrived at experimentally and others arrived at using the second science, namely, a situation similar to the one prevailing in physics and

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engineering. This kind of imaginary mathematics would have a weaker logical foundation than ours but, because experimentation there plays a more important role than in our mathematics, it is likely that many mathematical phenomena unknown or barely touched upon by us would be quite deeply understood by those imaginary mathematicians.

The way we are conditioned at present, there seems to be no chance that such an imaginary mathematics will take over. However, we may wish that we had at our disposal the highly developed experience in experimenting with mathematics the above imaginary civilization has and the many observations they have made. This could have greatly helped us in our own conventional mathematics. Now, there is nothing to prevent us from achieving such experience and making such observations if we seriously apply ourselves to developing *a science of experimental mathematics*, a subfield of mathematics (and/or computer science) which could occupy a status similar to that of, say, operations research.

Using present day hardware and software of computers, such a science could be of tremendous help in the development of both pure mathematics and the physical sciences. Again, experimental mathematics has always existed and is constantly practiced in one way or another by many or most mathematicians in conceiving, developing and perfecting new and old theories. But if it became more explicit, considered a science in its own right and had its own scientific vehicles, it would probably be of far more service than it has rendered up to now.

4. The following speculation indicates that experimental mathematics, whether organized into an independent science or just left to the devices of its individual practitioners, may play a significant role in days to come.

The recent proof of the four color conjecture indicates that it is likely that the use of computers will become an integral part of more and more proofs of theorems. It is reasonable to envision that eventually computers will be widely used not merely for numerical computations but also to carry out the logical steps of proofs. Furthermore, a day may come when not only proofs, but even the statement of many theorems will become so involved, that they could be handled by computers only; in fact, they will make no sense to a mathematician trying to understand them without mechanical aid. Many then will use the machine as almost a complete substitute to the human mind and argue that this is just a natural extension of numerical computation by machine which no one seems to object. But others may rebel claiming that a string of symbols can be considered a genuine piece of mathematics only if it is understandable by a human being without mechanical help. It is quite possible that at that time a deep split will occur in mathematics, much deeper than the one caused by the foundation crisis of the early part of this century. Mathematics could break into several sciences with different criteria for the validity and importance of mathematical results.

At that time, experimental mathematics may become one of the few bridges connecting the various factions and hence a very substantial organ in the feuding body of mathematics. For, by virtue of its methods, it will likely be very much in line with those heavily relying on computers in all phases of their mathematical doing. On the other hand, the more "purist" factions will live in peace with experimental mathematics as it does not claim to firmly establish mathematical theories but merely to be an aid to mathematical research by making plausible conjectures and indicating promising avenues of research on the basis of experiments and, of course, by occasionally settling an outstanding problem via a counterexample.

5. To make this discussion more concrete let us illustrate it with an example of a recent mathematical experiment. It is from linear algebra.

Consider a (real) positive definite Toeplitz matrix R,

$$R = \{r_{|s-t|};\, s, t = 1, 2, \ldots, n\}.$$

Form the inverse R^{-1} and the vector $v = R^{-1}e$ where $e = \mathrm{col}(1, 1, \ldots, 1)$.

It had been observed empirically in many cases that the resulting vector v had positive components only. The size of n was around 25. This led to the conjecture that v always has nonnegative entries only.

To settle this question some analysis was done and we found that if R is circulant, the conjecture is true. We did not succeed, however, in proving it in general.

Finally we turned to heuristic search. To get a better understanding of how the vector v varies with R we carried out a computer experiment in which the matrix R was picked "at random."

A technical difficulty in this connection is that it is not so easy to pick such matrices R "at random." We want them to be symmetric, which is easy, and Toeplitz, also easy. They also have to be positive definite which is a property further away from our intuition than, for example, symmetry. One necessary and sufficient way of verifying this property (there are lots of others, equally unattractive) is to use *Sylvester's criterion*:

$$\det(R_1) > 0,\ \det(R_2) > 0, \ldots, \det(R_{n-1}) > 0,\ \det(R_n) > 0,$$

where each R_k stands for the leading $k \times k$ principal submatrix of R. Determinants are notoriously clumsy to work with, both analytically and computationally, so that instead of generating symmetric Toeplitz matrices "at random" and selecting those that satisfied Sylvester's criterion, *we* *generated them directly by Carathéodory's representation of (finite) Toeplitz positive definite matrices* $\{r_{st}\}_{r,s=1}^{n}$:

$$r_{st} = \sum_{k=1}^{n} f_k \cos \lambda_k(s-t),$$

where $f_k > 0$, $0 \leqslant \lambda_k \leqslant \pi$ and the λ_k are distinct. We generate the f's as independent identically random distributed variables from a rectangular distribution over (0, 1) and similarly the λ's over $(0, \pi)$. The block in the flow chart (see Fig. 1) doing this is called CARATHÉODORY.

This procedure of generating positive definite matrices directly speeded up the algorithm considerably. We then compute v and test whether all entries are nonnegative. If a negative value is found, the program stops. Otherwise, it adjusts the λ-vector as in Fig. 2. The block ADJUST computes the criterion

$$M = \min_k v_k$$

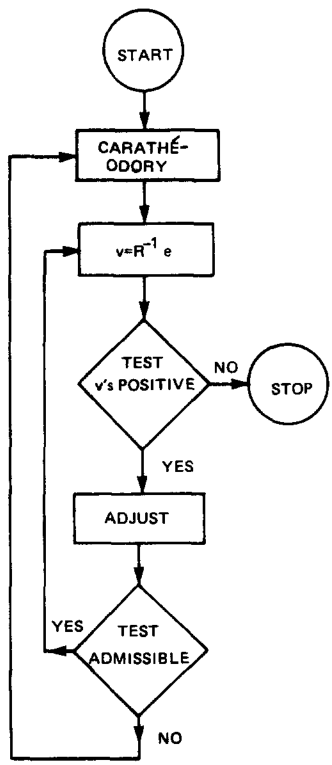

FIGURE 1

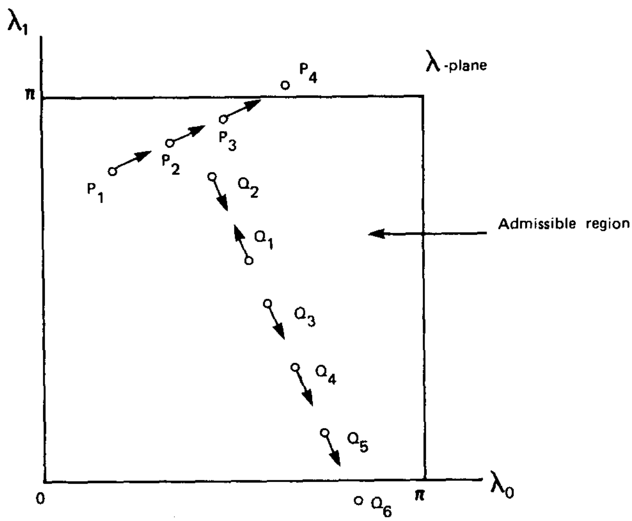

FIGURE 2

for two points, say P_1 and P_2 in λ-space. We then move by successive steps in the direction of decreasing M, along a straight line, until we get outside the set of admissible λ-values when we start over again, generating two new λ-points at random.

Of course the λ-values outside the region are not really inadmissible (periodicity!), but we do not want to keep them fixed indefinitely, so it seems wise to change them. A trajectory in λ-space can then look like P_1, P_2, P_3, P_4. It can also change direction as in the trajectory $Q_1, Q_2, Q_3, Q_4, Q_5, Q_6$.

As a modification of this strategy we also varied the f-vector linearly until some component became negative. We then had a $2n$-dimensional phase space.

Using the interrupt feature, we can stop the program at any time and print out R, R^{-1}, v or M to give us an idea of what is going on. Notice that *we do not use an entirely random search* in our $2n$-dimensional phase space; that would be very inefficient. *Nor do we use an entirely systematic search*, which would be near impossible, at least in higher dimensions. Instead, a combination of both seemed right.

Executing the program for $n=5$, about 30 iterations produced no negative M. We noticed a few cases of v-values close to zero, however. For $n=4$, about 100 iterations produced no negative v's and we did not even find any close to zero. For $n=3$, however, after about 30 iterations the program stopped and produced a matrix for which v had a negative entry: *the conjecture had been disproved!*

To gain some more experience for other values of n, we then returned to $n = 4$ where about 300 more iterations finally produced a counterexample and to $n = 5$ where 30 more iterations also gave a counterexample. There was some evidence that a purely random search would have been wasteful.

Armed with hindsight, it is easy to see what we should have done from the beginning: just evaluate the determinants needed for $n = 3$ and let the six variables vary, while keeping the matrix positive definite. We finally carried out the boring and time-consuming, but perfectly elementary, algebraic manipulations. We found, indeed, that there is a nonempty set of matrices R satisfying the conditions and with at least one negative v-entry. The set is thin, which is why we did not find it earlier during the experimentation.

Before we had the result of the heuristic search, it seemed futile to do this exercise in algebra since the result would probably not have been conclusive and larger values of n would be too cumbersome. *We had been almost sure that the conjecture was correct so that our main effort went into unproductive attempts to prove it rather than look for exceptions.*

The programming of the search algorithm in APL took about one hour (to design the algorithm took longer, of course), debugging 30 minutes and execution 20 minutes connect-time, all done interactively. The CPU-time needed was negligible.

This computational experiment is an example of how the mathematician can exploit the computer as his laboratory to explore hypotheses and use it as a research tool supplementing the traditional deductive method.

We also learned from this experiment that the heuristic search could be made fairly fast, certainly better than purely random or purely systematic search, by employing the analytical structure of the setup, in this case, Carathéodory's theorem.

This example and the figures are from [1] where more details and many other experiments are reported.

Reference

1. Ulf Grenander, "Mathematical Experiments on the Computer," Academic Press, New York, 1982.

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