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Popperian geophysics and tunnelling algorithm

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Abstract. Parasnis has observed in a presidential address that geophysics is not a Popperian science in a major way. That is, hypotheses are not consciously put forth in a falsifiable format and much of the effort goes in seeking supporting evidence for favoured hypotheses. Parker evolved a parameter extremization strategy, initially to tackle the problem of non-uniqueness in geophysical inference. Later he based a hypothesis testing proposal on it, which is refreshingly Popperian. It has not been adopted widely, partly because it requires global extrema, and not local and this has been regarded as a problem with no solution. Attention is drawn towards tunnelling algorithm, which solves the problem of global optimization successfully, makes Parker's Popperian proposal practical and extends the range of Popperian geophysics.

Keywords. Popperian geophysics; tunnelling algorithm; Popper's demarcation criterion; Parker's theory; non-uniqueness in geophysical inference; local minimum syndrome.

1. Introduction

This paper deals with three important ideas: Popperian criterion of science, hypothesis testing in geophysics in the face of non-uniqueness in inference from data and global optimization algorithms, in particular, the tunnelling algorithm. It was believed universally till recently that it was not possible to prove that the extremum obtained was global and not merely local when the problem was multiextremal. In view of the progress in the field of multiextremal optimization, there is no more reason to have this "local minimum syndrome". Parker (1977) made a powerful suggestion of how extrema of a chosen functional of model parameters, derived from the observations, could be used to disprove some geophysical hypotheses. But the procedure requires global extrema and not local ones. As global optimization methods were not a part of geophysical folklore then or even now, the procedure was never seriously used as it deserved to be. That difficulty is no more there. Therefore, Parker's scheme could be used to definitely reject some hypotheses though others may not be conclusively proved. That, indeed, is the central notion in Popperian science. As philosophy of science is not as widely read as it should be, a brief introduction to Popper's criterion of demarcation of science from other intellectual endeavours is offered. Parker's proposal is then described as an interesting application of a Popperian attitude to geophysics. Then the local minimum syndrome that affects the geophysical practitioners, and surprisingly enough, even the mathematicians is illustrated and its outdatedness is suggested by describing tunnelling algorithm for global optimization. The purpose is to suggest worthwhile applications for that algorithm, strengthen Parker's parameter extremization approach to deal with non-uniqueness in geophysical inference, make geophysical practice more scientific by adopting hypothesis testing and spread Popperian attitude by emphasizing that it is really practicable even in a field like geophysics in which frequently the data seem to be inadequate to resolve the theoretical issues.

2. Popper's demarcation criterion

Every logical argument is not scientific. Science deals with the external, empirical world and, therefore, empirical facts are the arbiters of our hypotheses about the world. An attempt can be made to look for an ever-enlarging support in the external world for the preferred theory. But it is, indeed, futile as any set of postulates with a built-in contradiction can explain everything (Popper 1968, p. 91). In fact, that is what metaphysical hypotheses do.

Therefore, one should pay heed to an asymmetry in deductive logic: Any amount of empirically verified deductions is unable to establish the hypothesis, whereas a single false deduction from the hypothesis about the external world is enough to disprove the hypothesis (or at least one postulate in it). This prompted Popper to propose that the true hallmark of scientific theories is testability and falsifiability and not verifiability (Popper *loc. cit.* p. 40). Thus, the proposer of a theory should indicate the empirical conditions under which he is willing to abandon the theory. Rather, the theory should be articulated with such clarity and precision that anyone, following deductive logic, would be in a position to derive many material and testable implications of the theory, it being understood that any of these implications empirically proved wrong automatically disqualifies the theory and establishes the need for a better theory. The objective is not to improve the longevity of an adopted theory by protecting it (Popper *loc. cit.* p. 54) or to seek support for it, but to select one which is the fittest to survive under persistent falsifying attempts (Popper *loc. cit.* p. 42). Science, thus, is not a corpus of established and accepted results, but is a method. The importance of method in science is supreme. "Once the method is learned... men's wits are levelled; any one can do science", wrote Hesse (1964). The method rejects what is empirically disproved and hopes to further test everything that is not yet so disqualified.

With its emphasis on falsifiability and refutability as hallmarks of science Popper's criterion of demarcation has come to be criticized as negative. While stressing that this negative criterion is indeed the essence of scientific method, Popper (1984, pp. 242–248) has also conceded the importance of some positive considerations if science is not to stagnate and has also suggested various indices for the growth of scientific knowledge (Popper 1984, pp. 215–292, pp. 385–413). Even during this discussion he has, however, emphasized that a scientific hypothesis should have a high content or verisimilitude and not high probability of being true, as the latter would mean low content. Important as this point is, it has no direct relevance to the present theme.

Popper's criterion is a proposal (Popper 1968, p. 37) and does not enthuse everybody. According to Curry (1965) it is not even proper to characterize any science by demarcating its circumference. He suggests that the proper attempt is to define the central core or the heart of a science and let the boundaries take care of themselves. Lakatos (1978) points out that facts cannot be judges of theories, because F being a veridical fact is itself a theory and, therefore, we essentially have a clash between theories to be resolved. Popper (*loc. cit.* p. 107) counters by suggesting that the experimental results being interpretations based on believed theories is, all the more, a reason why verification of a theory is always easy to arrange, justifying critical attitude advocated by him. Further, he accepts a particular experimental result as a falsifier only if it is embedded in a reasonable theory, as science is concerned with theories and not stray facts. Peirce (1957) opined that "the method" of science cannot be prescribed once for all, as it must also evolve as science evolves. Popper's criterion of demarcation has, indeed, evolved out of criticism of earlier criteria which brought out their inadequacy. His criterion of falsifiability obviously implies his willingness to abandon it if its shortcomings are brought out. Yet at the present state of evolution of science the normative Popperian demarcation of science seems to be very satisfactory. Moreover, his criterion is open. A hypothesis may be unfalsifiable when it is put forward and, hence, unscientific in a Popperian framework. But when newer experimental techniques develop, it may become falsifiable (Quinton 1964) and, hence, scientific. The same role may be played by newer falsifiability strategies, as is illustrated in the next section. Thus, the demarcation achieved by Popper's criterion is dynamic and the scope of science under it progressively widens.

There are other competing philosophies of science from different perspectives. Kuhn's (1970) historical or sociological philosophy, in particular, has many adherents. Inappropriateness of using history to define a desideratum such as science has been adequately argued (Brush 1974).

However, philosophy of science is a highly opinionated field. The debate between Popperians and Kuhnians is particularly acrimonious. That debate is not relevant to the theme of the present paper. Earth scientists tend to lean more on Kuhn or subsequent revisions of his paradigm (see e.g. LeGrand 1988) such as Laudan (1977, 1984) and ignore or underrate Popper (see e.g. Halstead 1980). The relevant aspects of this phenomenon are discussed elsewhere (Moharir, to be published, a). At present, Popperian criterion is adopted and it is shown that some recent developments in mathematics can enlarge the domain of Popperian geophysics. It may be rather redundant and yet useful to point out that to adopt a model is not the same thing as assuming that there are no problems in it or that it cannot be improved upon. Sociologists of science (see e.g. Laudan 1984) should readily agree. Inadequacy of Popperian criterion has been dealt with by the present author elsewhere (Moharir 1992a, b). What is incomplete can also have a strong core of value, as is certainly true about the Popperian criterion of demacration. Hence the present exercise of suggesting a possibility of its application to geophysics.

3. Non-uniqueness in geophysical inference and Parker's proposal

The non-uniqueness in geophysical inference from observations is widely recognized. This makes the task of testing and falsifying theoretical predictions rather difficult. In the context of linear models, Backus and Gilbert (1970) have suggested looking for model averages which are shared by all the data-compatible models. Parker (1974, 1975, 1977) retained this notion of determining the common properties of all the permissible models even for the nonlinear case and advocated the use of upper and lower bounds on a prescribed nonlinear functional of model parameters for the purpose. This is a more manageable problem than specifying the entire class of feasible solutions and yet is important in its own right. In the case of gravity data, it leads to ideal body solutions (Parker 1974, 1975; Ander and Huestis 1987) which are unique and are readily obtained. But, in general, a nonlinear multiextremal optimization problem results and Parker (1977) observed that "it is almost impossible to show rigorously that a global extremum has been found, not merely a local one".

Apart from its potential to characterize non-uniqueness, a very important use, suggested by Parker (1977), of his strategy of parameter extremization is in testing geophysical hypotheses. A hypothesis is an idea or a conjecture of a geophysicist, prompted by analogy, extrapolation, or suggestive evidences. A bound on some property (e.g. mean acoustic velocity in a prescribed depth interval or S-wave attenuation) may be derived from the hypothesis, with a view to characterize what it requires. Then, an inverse problem is solved to convert the appropriate empirical measurements to obtain extreme bounds on the same property to decide what the data rule out. Then, if the hypothesis requires what is excluded by the data, the former *must* be rejected, otherwise it *may* be true. As Parker (1977) wrote: "Naturally the test cannot prove the correctness of the model, but it may be able to reject it." That is precisely a Popperian attitude.

In his presidential address, Parasnis (1980) lamented that geophysics is not yet a Popperian science in a major way. Parker's proposal is sound in principle and has already been adopted by Gubbins (1975) and Jordan (1975), among others. Yet it has not been utilized as extensively as one would have desired, possibly because (a) its methodological appeal has not been recognized by some due to want of explicit exposure to philosophy of science, and (b) it requires global extrema and not local ones, and this objective was seen to be difficult to guarantee.

Even attracting the charge of stating the obvious, it may be added that not every problem in geophysics has non-uniqueness for the same reason, Parker's solution to that problem is not the only one (Moharir 1990), not every question in geophysics involves mathematical extremization, etc. But there is an important subset of geophysical problem formulations wherein these are the ruling concepts and the suggestion in this paper pertains to that subset.

4. Local minimum syndrome

Optimization problems are of ubiquitous occurrence. The iterative procedure designed to solve the optimization problem should be terminated when the optimality conditions are satisfied. Unfortunately, these conditions are generally merely necessary and not sufficient conditions, unless the problem is convex. Therefore, it is not easy to decide whether the global optimum has been reached (Jacoby *et al* 1972). Till recently, the strategy proposed was to initiate the computations at many different initial guesses and verify whether the same terminal solution is obtained (Jacoby *et al* 1972; Ray and Szekely 1973; Burley 1974). Even if such a thing happened, the doubt would still persist. This local minimum syndrome was ubiquitous even in the books on optimization. "All the methods discussed in this book... perform searches for local minima", declared Aoki (1971). Another book (Dennis Jr. and Schnabel 1983) admitted that "...when a local minimum is reached there is not much one can do except report what has happened and advise the user to restart elsewhere". Powell (1982) suggests that "convergence to a local rather than global solution would be expected", records "accelerating progress in the methodology for finding local optimum solutions", and recommends that even though "global optimization should not be discussed as an unrealistic aim", "solution methods must exploit simplifying features even in one or two dimensions" These excerpts are representative of the general attitude in mathematical books on optimization proper, always till the first half of the 1970s, and surprisingly even later, when some imaginative and successful global optimization methods had already been developed (see § 5) by the researchers and hence a change of paradigm was due.

There is no wonder that geophysicists, barring few exceptions which are growing in number (Rothman 1985; Landa *et al* 1989; Khattri *et al* 1987; Sastry and Moharir 1990; Dossa and Oldenburg 1991) are still under the influence of the local minimum syndrome. Wiggins (1978) suggested the notion of minimum entropy deconvolution of seismic traces and borrowed varimax norm for simple structure from the field of factor analysis and maximized it. Others quickly picked up the notion and used many alternative simple-structure norms (Ooe and Ulrych 1979; Gray 1979; Donoho 1980; Cabrielli 1984; Teotia 1985). Wiggins (1985) summarized the performance of these schemes as unsatisfactory and identified the multi-extremal propensity of simple-structure norms as one of the causes for failure. He was, however, not aware that there is now no difficulty in obtaining global extrema. Even more recently, Mora (1989) observed that "...inversion schemes...may converge to local minima...avoided by starting with a...model that is sufficiently close to the solution". "Except for experimentation with a variety of initial guesses (which is usually inconclusive since one can never examine enough), there is no general method for determining whether a solution obtained by the iterative method really does minimize error in the global sense", concluded Menke (1989).

When a problem eludes solution for too long a time it gets accepted as not only a difficult but an impossible one. Then when a solution is obtained, it is not even noticed for a fairly long duration. This is what has happened in the case of global optimization problem. But now that some solutions are available, Parker's Popperian proposal should be exploited in many ways.

5. Tunnelling algorithm

One of the methods of global optimization, called simulated annealing was proposed by Kirkpatrick *et al* (1983) and extended by Bohachevsky *et al* (1986). It has been employed in geophysics by Rothman (1985), Landa *et al* (1989), Dosso and Oldenburg (1991), etc. But it is a statistical method, the escape from a local extremum being only statistical. Another method called the controlled random search has been developed by Price (1978) and used in geophysics by Khattri *et al* (1987). It too is essentially a clever adaptation of a Monte Carlo scheme. A tunnelling algorithm (Levy and Montalvo 1977, 1985; Montalvo 1979; Levy *et al* 1982; Gomez and Levy 1982; Levy and Gomez 1980, 1985) to be described here is a deterministic scheme which moves to the global extremum systematically through a sequence of extrema, each progressively better than the previous one. It has some ancestry (Goldstein and Price 1971; Treccani 1978) but it stays clear of the limitations and difficulties of these earlier deterministic methods. A variation of it was used for a geophysical application earlier (Sastry and Moharir 1990).

Let $f(\mathbf{x})$ be a function whose global minimum is to be found out. The basic idea of a tunnelling algorithm is as follows: Start at a point $\mathbf{x}_1^0$ and from there reach a local minimum $\mathbf{x}_1^*$. Then somehow reach another point $\mathbf{x}_2^0$ such that $f(\mathbf{x}_2^0) \leqslant f(\mathbf{x}_1)$. Obviously $\mathbf{x}_2^0$ can be a starting point for a new local minimization phase, which will lead to a lower local minimum. This phase of going from a local minimum to another point which will lead to a lower local minimum (if any) is called tunnelling. The tunnelling algorithm thus operates by alternating phases of local minimization and tunnelling, generating a sequence of points $\mathbf{x}_1^0, \mathbf{x}_1^*, \mathbf{x}_2^0, \mathbf{x}_2^*, \ldots \mathbf{x}_i^0, \mathbf{x}_i^*, \ldots$ wherein $\mathbf{x}_i^*$ is a local minimum and $f(\mathbf{x}_j^0) \leqslant f(\mathbf{x}_{j-1}^*)$. Tunnelling is the crux of the algorithm and is achieved as follows. Suppose a tunnelling function

$$T_0^{(i)}[\mathbf{x}, f(\mathbf{x}_i^*)] = f(\mathbf{x}) - f(\mathbf{x}_i^*) \tag{1}$$

is defined. Then $\mathbf{x} = \mathbf{x}_i^*$ is its zero, but it possibly has other zeroes. Any one of them could be taken as $\mathbf{x}_{i+1}^0$, because then $f(\mathbf{x}_{i+1}^0) = f(\mathbf{x}_i^*)$ or one has moved or tunnelled away from the local minimum $\mathbf{x}_i^*$. Thus, tunnelling is achieved by finding a zero of the tunnelling function. But $T_0^{(i)}$ has a drawback as a tunnelling function, because $\mathbf{x}_i^*$ is also a zero and the zero-finding algorithm may be attracted towards it. Therefore, this zero must be destroyed. This is readily done by modifying $T_0^{(i)}$ to

$$T^{(i)}(\mathbf{x}, \mathbf{t}_i) = \frac{f(\mathbf{x}) - f(\mathbf{x}_i^*)}{[(\mathbf{x} - \mathbf{x}_i^*)'(\mathbf{x} - \mathbf{x}_i^*)]^{m_i}}, \tag{2}$$

where $\mathbf{t}_i$ is the tunnelling parameter vector

$$\mathbf{t}_i = [\mathbf{x}_i^*, m_i, f(\mathbf{x}_i^*)] \tag{3}$$

and the superscript prime denotes transposition. The denominator in equation (2) introduces a pole of strength m_i at $\mathbf{x}_i^*$. The strength m_i is adjusted to be just larger than the mutliplicity of zero of $T_0^{(i)}$ at $\mathbf{x}_i^*$, so that it is adequately annulled. Now the zero of $T^{(i)}$, if any, will give $\mathbf{x}_{i+1}^0$ at which the next local minimization phase begins. Obviously, every time a new local minimum is reached, the tunnelling function is redefined according to (2).

A complication arises when the point $\mathbf{x}_{i+1}^0$ reached by tunnelling is itself a local minimum, i.e. $\mathbf{x}_{i+1}^*$. Then, if the tunnelling function $T^{(i+1)}$ is defined according to (2) to annul the zero at $\mathbf{x}_{i+1}^* = \mathbf{x}_{i+1}^0$, the earlier local minimum $\mathbf{x}_i^*$ will still be a zero and the zero-finding algorithm may lead there. Therefore, to ensure that the sequence $\mathbf{x}_1^*, \mathbf{x}_2^*, \ldots$ has a past-avoiding property, the tunnelling function is defined to be

$$T^{(i)}(\mathbf{x}, \mathbf{t}_i) = \frac{f(\mathbf{x}) - f(\mathbf{x}_i^*)}{h_i h_{i+1}}, \tag{4}$$

if

$$\mathbf{x}_{i+1}^0 = \mathbf{x}_{i+1}^*,$$

where

$$h_i = [\mathbf{x} - \mathbf{x}_i^*)'(\mathbf{x} - \mathbf{x}_i^*)]^{m_i}, \tag{5}$$

so that a pole of adequate strength m_{i+1} at $\mathbf{x}_{i+1}^*$ is introduced, in addition to the pole of strength m_i at $\mathbf{x}_i^*$. The tunnelling parameter vector $\mathbf{t}_i$ is now

$$\mathbf{t}_i = (\mathbf{x}_i^*, m_i, f(\mathbf{x}_i^*), \mathbf{x}_{i+1}^*, m_{i+1}). \tag{6}$$

It is immaterial whether the numerator is written as $f(\mathbf{x}) - f(\mathbf{x}_i^*)$ or $f(x) - f(\mathbf{x}_{i+1}^*)$, because in the present context $f(\mathbf{x}_i^*) = f(\mathbf{x}_{i+1}^0) = f(\mathbf{x}_{i+1}^*)$. This is also the reason why $f(\mathbf{x}_{i+1}^*)$ is not shown as an argument in $\mathbf{t}_i$ in (6). There may be more than two local minima at the same level and the past-avoiding strategy is an easy generalization of (4). The tunnelling algorithm can thus take care of several local (and similarly global) minima at the same level. That is the situation where the algorithm of Treccani (1978) had floundered. It is reported (Levy and Gomez 1985) that a case of even 18 coeval minima was successfully handled by the tunnelling algorithm. As soon as a local minimum at a lower level is reached again, the simplicity of the tunnelling function of (2) is restored.

In the tunnelling algorithm the computational effort does not go up in proportion to the number of minima, as it does not encounter all the local minima. Also, the curse of dimensionality (Bellman 1961) does not operate very seriously for this algorithm. This can be readily appreciated by a comparison of two problems among many reported by Levy and Gomez (1985). A ten-dimensional problem with 10^{10} local minima needed an average time of 68·22 s, the average being taken over the various initial guesses $\mathbf{x}_1^0$. On the other hand, a two-dimensional problem with 760 local minima needed an average time of 87·04 s, because it had 18 coeval local minima, the situation which makes the tunnelling algorithm inefficient. For the latter problem, when the 17 extra coeval minima were removed, the average time required came down to 8·47 s.

Finding a zero of multidimensional tunnelling function is a relatively difficult problem. It has now been greatly simplified (Yao 1989).

Again, for the sake of completeness, it is good to be aware that the tunnelling algorithm is not the ultimate in optimization. Menke (Personal communication) pointed out that it may fail when there are infinitely many coeval local minima or when local minima are not discrete points but are hypersurfaces. Another referee has pointed out that the tunnelling algorithm will fail in infinite-dimensional spaces. So, it must be shown that the true solution to extremization resides in a finite-dimensional space or that a sequence of finite-dimensional solutions converges to the true solution. He reminds that these are really hard problems. These observations are true, but so are they about optimization without tunnelling algorithm. So some problems still remain or would always remain, but on that background tunnelling algorithm still constitutes a progress, which is not nullified by persistence of problems and pathologies.

6. Discussion

With a good global optimization algorithm now available, parameter extremization of Parker can be performed and his hypothesis testing proposal in the Popperian vein can be adopted. This will help towards furthering the realization of Parasnis's presidential dream of Popperian geophysics, widening its range by opening a new falsification strategy.

Stating the obvious, there are other possibilities and methods of furthering geophysics as a Popperian science. Some of them have briefly been dealt with elsewhere (Moharir 1988, 1990). Yet that problem remains unattacked in a major way, because Popperization of science is not an easy objective, nor is it always an objective of working scientists (Laudan 1984; Le Grand 1988; Rudwick 1985; Secord 1986; Oldroyd 1990). So what has been suggested here is a modest proposal and not a comprehensive solution to Popperization of geophysics.

Tunnelling algorithm or any other global optimization method such as the simulated annealing is a development in mathematics which has applications in scientific disciplines using optimization, and not only in geophysics. For example, simulated annealing has been frequently used in and outside geophysics (Szu and Hartley 1987; Farhat and Bai 1987; Benvenuto and Marchesi 1989; Schneider Jr and Whitman 1990; Runge and Runge 1991; other references cited earlier). The author considers tunnelling algorithm to be superior and finds that it is not mentioned in surveys on global optimization (Manetsch 1990; Pardalos and Rosen 1986, 1987). One aim of the paper has been to bring this deterministic algorithm to the notice of the prospective users. The restriction to geophysics is entirely due to the professional affiliation and the journal of publication though slightly more importantly that is also an area in which furthering Popperization is more essential.

A more important purpose of the present paper is to point out that the developments in global optimization have deeper implications than merely solving optimization problems in science more satisfactorily. Obviously, there is much in geophysics which does not fulfil Popperian demarcation criterion. It is of interest to see whether the difficulties, as many of them would not be insurmountable, can be overcome. The paper does not deal with everything that needs be done to make geophysics qualify as a Popperian science. It merely deals with one specific suggestion, as should be clear from the title. The presently non-feasible testability of a hypothesis pertaining to the empirical world could graduate into feasibility due to (a) a new measurable property being defined, (b) a new measurement technique emerging, (c) a new mathematical theorem leading to newer implication of the hypothesis which could be testable, (d) a new numerical technique or a mathematical algorithm converting a problem previously regarded as insolvable into a solvable one, (e) a new phenomenon being discovered which together with its laws has implications for the hypothesis under consideration, (f) a new experimental or observational technique becoming available, and so on. Study of the empirical world involves a complex interaction among hypotheses, techniques of measurement, logical and mathematical theorems and experimental techniques. New developments in any one of these areas could have new implications for the testability of hypotheses. This paper deals with the emergence of tunnelling algorithm which has made a previously intractable problem of global optimization soluble. There obviously are some inferences about the empirical world which are stated in terms of bounds on some properties, requiring such a solution of the global optimization problem. When this problem was intractable, these inferences were not testable, but now they can become testable. This is a clear case of development in mathematics having implications in empirical fields, which should not be surprising at all, because it has been happening all the time. Yet a doubt has been raised by a referee how a 'technical' development such as a new algorithm, however useful it may be, may help to solve a 'philosophical' problem. There is an unnecessary ordination here, implying that everything 'technical' is at an unimportant level, it may be useful but cannot contribute significantly to problems at higher levels of science and philosphy and that only some deeper and broadbased considerations should be meaningful at the latter levels. He sees a certain lack of proportion or appropriateness in the case made by this paper, but actually the expectation of proportion between a cause and the effect, a trigger and the released consequences, a facility and its utility, a method and its applicability, origin and subsequent development, itself is fallacious. Possibly, the word 'algorithm' has played a depreciatory role. Tunnelling algorithm is not an algorithm; nomenclature apart, it is a concept which does not prescribe any specific numerical techniques for its implementation. It is not a way of solving a problem which had other known techniques available to solve it, such that what has been achieved is only a secondary pragmatic advantage such as efficiency, reduction in computational effort, simpler book-keeping or storage management. It is a new concept which leads to the solution of a problem which was otherwise taken to be unsolvable. The referee's doubt and the feeling of lack of proportion are, therefore, misplaced.

Those who prefer simulated annealing and/or controlled random search for global optimization can achieve the same objective with those methods as has been proposed here in the context of the tunnelling algorithm. The experimental evaluation of these methods is also not completed (see e.g. Johnson *et al* 1989).

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