PHILOSOPHICAL TRANSACTIONS OF THE ROYAL SOCIETY A
MATHEMATICAL, PHYSICAL & ENGINEERING SCIENCES

A Problem in the Application of Inverse Methods to Tracer Data [and Discussion]

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Phil. Trans. R. Soc. Lond. A 1988 **325**, 85-91
doi: 10.1098/rsta.1988.0044

Phil. Trans. R. Soc. Lond. A **325**, 85–91 (1988) [85]
Printed in Great Britain

A problem in the application of inverse methods to tracer data

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Attempts to apply inverse methods to the interpretation of tracer data usually seek some least squares solution of the flux divergence equations

$$\boldsymbol{A}\boldsymbol{C} = \boldsymbol{S},$$

where A is a matrix of transport coefficients, $\boldsymbol{C}$ a vector of concentrations and $\boldsymbol{S}$ a vector of sources/sinks.

However, what is often really required is a set of values for the elements of A, which will give a satisfactory prediction of the concentrations. This corresponds to finding a least squares solution of

$$\boldsymbol{C} = A^{-1}\,\boldsymbol{S}.$$

The two problems are not equivalent. The latter corresponds to an extensively re-weighted version of the former, where the weights depend on the solution (the elements of A). The former is linear in the elements of A: the latter is highly nonlinear. In addition, the matrix A is invariably sparse, and required to be so. However, A^{-1} is not, nor is it guaranteed that its inverse will be if its elements are determined freely.

It is not clear whether the standard methods of generalized inverse theory are applicable to the more difficult 'real' problem nor, if they are not, what other methods might be used. It is, however, possible that solutions of the 'real' problem, if they can be found, would be more informative.

1. Introduction

The application of inverse methods to the interpretation of oceanic geochemical and hydrographic data, with a box model representation of the system, was pioneered by Wunsch & Minster (1982). On the face of it this methodology is ideally suited to the problem. Box models have been used for many years by chemical oceanographers to describe the systems of interest to them (see, for example, Broecker 1979; Keeling & Bolin 1967). The systems of equations involved are not large, and the transport processes are very naturally represented by the set of linear equations that arise.

The success of attempts to use this technique is difficult to judge, because the truth is not usually known. In general, however, those who have tried it seem to have been less than satisfied with their results, either because the solutions contained implausible features, or because the results revealed inconsistencies between the data and the model (Schlitzer 1984; Bolin *et al.* 1987; Mobbs *et al.* 1987). In addition simulation studies (Fiadeiro & Veronis 1984) have revealed that the solutions may be very sensitive to the details of the technique. Although it is true that inverse methodology also permits much information about the indeterminate features of the solution to be obtained (Wunsch 1985), its interpretation is not entirely straightforward. There are several possible reasons why work in this field has not been as productive as had been hoped.

First, it seems likely that we have been attempting to determine too much from tracer data alone. Asking for advection and diffusion to be determined at every interface requires the determination of small-scale features, and may anyway lead to structural indeterminacy. It is after all well known that even in a simple one-dimensional system only the ratio of advective and diffusive transports can be deduced from steady-state tracer data, and not both quantities independently.

Second, obtaining realistic solutions from under-determined systems requires that the auxiliary information used (e.g. choosing the norm to be minimized in constructing a generalized inverse) be well-chosen. This may not be straightforward.

Third, some care is needed to ensure that the mathematical problem is a proper representation of the practical or intellectual problem of interest. It is this aspect that I wish to discuss in this paper.

2. Forward, reverse and inverse problems

The systems of interest are fluids in which the processes of advection and turbulent diffusion interact, and where various tracers are created and destroyed by sources and sinks. The mathematical description is based on the classical differential equation

$$dC/dt = \operatorname{div}(K \operatorname{grad} C - uC) - \lambda C + S, \tag{1}$$

where C is the concentration of a tracer, K represents turbulent diffusivity, u the velocity field, λ a decay rate (chemical or radioactive) and S other sources or sinks.

For convenience in fitting to available data this equation is usually applied to a finite representation in the form of a (not very large) number of boxes: this is equivalent to the use of a rather coarse finite-difference or finite-element representation. Concentrating for simplicity only on the steady-state problem, it is easily shown that (1) may be reduced to a set of linear equations

$$\sum_j A_{ij} C_j = -S_i, \tag{2}$$

where there is one value of C and one of S for each box (i.e. both i and j index boxes). The elements of the (square) matrix A_{ij} are transport (exchange) coefficients, consisting of a diffusive and an advective element. They have the dimensions of volume transport rates; the exact form depends on the discretization process (upstream, weighted or centred diffencing, etc.) adopted. The linear equations (2) may of course be written in matrix form

$$\mathbf{A}\mathbf{C} = -\mathbf{S}. \tag{3}$$

In what follows I shall for simplicity speak as though one were concerned with only one tracer field, and ignore the additional (but very important) constraints imposed by conservation of water. This captures the essence of the problem, because adding additional tracers does not alter the structure of the problem. Conservation of water is in any case probably best ensured by the technique of 'loops' (characteristic circulations) adopted by Bolin *et al.* (1987). It is also simpler (but not essential) to proceed as though the diffusive transports were known or specified.

Mechanistically, the concentration field (approximated by the vector $\mathbf{C}$) is produced by the transport processes (represented by the matrix A) working on the field of sources and sinks (the vector $\boldsymbol{S}$). Thus it is natural to regard the solution of (3) for the concentrations, for given A and $\boldsymbol{S}$, to be the forward problem, corresponding to

$$\boldsymbol{C} = -A^{-1}\,\boldsymbol{S}. \tag{4}$$

Note that (confusingly) the forward problem involves the inverse of A.

In interpreting tracer data, what is usually required is to determine the unknown elements of A, for given values of $\boldsymbol{C}$ and $\boldsymbol{S}$. This is the inverse problem.

The usual procedure for solving this inverse problem has been to seek least squares solutions of (3), i.e. to minimize the residuals of the flux-divergence equations. This is most conveniently done by rewriting the equations in the equivalent form

$$B\boldsymbol{W} = \boldsymbol{S}'. \tag{5}$$

Here B is a sparse matrix whose elements are concentration values, and $\boldsymbol{W}$ is a vector of the unknown transport coefficients. $\boldsymbol{S}'$ is a vector of sources and sinks, modified by decay (and diffusive flux divergence if diffusive exchanges are treated as known). Standard and very efficient methods for the solution of linear equations (e.g. singular-value decomposition) may then be applied, after appropriate attention to row and column scaling (see, for example, Wunsch & Minster 1982; Wunsch 1985). Note that the matrix B is not square, unlike A, and that it may be both underdetermined and inconsistent at the same time (Bolin *et al.* 1987).

This is a simple and efficient way to attack this inverse problem, but it is not the only way, and it may not be the best way. Firstly, the concentration and source/sink data are treated as exact: concentration values in particular are simply fed in as matrix elements, and analysis of the influence and propagation of errors in them is not straightforward. Second, minimization of residuals of the flux-divergence equations may not be the most appropriate goal. For many practical applications, one wishes to determine transport coefficients (i.e. the elements of the vector $\boldsymbol{W}$ or equivalently of the matrix A), to use them in a predictive mode. The goal is not just the interpretation of the data, but the construction of a model (essentially the box structure and a set of transport coefficients) that will have predictive utility. This is the situation when one is aiming to contribute to evaluating the problems of anthropogenic CO_2 releases, or radioactive waste disposal, for example (Bolin *et al.* 1987; Mobbs *et al.* 1987).

In these cases, a more appropriate goal would be to select transport coefficients that would yield solutions of the forward problem that fitted the data as closely as possible, i.e. to minimize the residuals of the forward equations (4), rather than the reverse (flux-divergence) equations (2), (3) or (5).

3. Nonlinearity

These statements of the problem are not equivalent. The forward version corresponds to an extensively reweighted version of the reverse version. In addition it is nonlinear in the unknowns (the non-zero elements of A). Finally, it is not obvious how it may be solved efficiently, especially if one recognizes that the elements of $\boldsymbol{S}$ cannot generally be treated as exact.

This problem was recognized by Wunsch & Minster (1982), who discuss it in §4.2 of their paper, and propose the use of the total inversion method of Tarantola & Valette (1982) (see also Mercier (1986)). This expands the size and complexity of the problem considerably, and may not be the ideal approach. Other methods are conceivable (Bolin *et al.* 1987).

The extent of the problem may be appreciated if one considers an obvious (but very unpromising) method; to solve directly for the individual elements of the inverse matrix A^{-1}. This preserves the linearity of the problem, but increases the number of unknowns to n^2 from (typically) $3n$ (for a three-dimensional configuration of n boxes). In addition, A is required to be sparse (only specified interconnections should exist), but there is no guarantee whatever that the inverse of A^{-1} (once it were determined) would be sparse. Ideally one would like to hold the number of unknowns at the number of non-zero transport coefficients, while guaranteeing the appropriate structure (sparseness and asymmetry) of A.

4. Analogies with linear regression

The problem is quite analogous to that of linear regression where, because the fitted line does not coincide with the data, there is an incidental variable (the fitted value) for each datum. It is possible, as in total inversion, to treat all these incidental variables as unknowns to be determined, subject to the constraints that all must lie on the fitted line. This is unnecessary in the regression problem, because its structure is such that one can determine the usual regression parameters independently, and simply compute the incidental variables afterwards. Alternative approaches to the problem may thus generate both large complex and time-consuming algorithms, or small, elegant and efficient ones.

The relation between inverse problems and regression was noted by Wunsch (1978), but does not seem to have received much attention since then. I suggest that it may be worthwhile to pursue the analogy, because there is a further parallel with regression, in that predictive regression is a linear problem, whereas functional regression (where one allows for errors in all variables) is nonlinear. Indeed, multiple functional regression may be reduced to an eigenvalue problem (Sprent 1969, ch. 6), which of course corresponds to the solution of a polynomial equation, but for which well-established algorithms, with alternative methods, are available. The full box-model inversion problem (allowing for errors in both C and S) may indeed be written as a multiple functional regression problem, and it would be of great interest to pursue this approach to its solution.

A further idea from statistics that may be relevant is that of the loss function. Physical scientists have a tendency to seek the 'true' solution to a problem (corresponding in many cases to a functional regression, for example). However, for practical purposes it may be desirable to use another loss function (i.e. the objective function to be minimized) such as mean square prediction error. This leads (in general) to different solutions, which are often 'shrunk' towards some mean value (see, for example, Copas 1983). In the box-model inversion problem, this might mean seeking models that minimize the prediction error for concentrations, rather than the 'best' physical transport coefficients.

It is therefore still possible that the disappointing results obtained from box-model inversions to date are in part caused by insufficiently developed methodology. As Wunsch has pointed out, the same problems arise in many fields and some methods have been re-invented several times. Work to date has been strongly influenced by geophysical techniques, but there are also results from the statistical theory of regression that may help us to find apt and efficient methods of solution for this most interesting class of problem.

I thank C. Wunsch for his criticism of my abstract, and for drawing my attention both to §4.2 of his 1982 paper, which I had forgotten, and to the work of Mercier.

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Discussion

W. J. Jenkins (*Woods Hole Oceanographic Institution, Massachusetts, U.S.A.*). It is my belief that the utility and potential of inverse calculations performed to date is not limited as much by technical issues associated with the computational 'machinery', as it is by the paucity of data and the appropriateness of the model geometry. As to the former, it is clear that there are simply not enough data to confidently answer the questions we are beginning to ask with such calculations. Regarding the latter, I feel that the geometry of the models used in such calculations, and the formulation of the constraint equations themselves have not been as well matched to the questions as they could be. In fairness to the modellers, the data limitations often force painful compromises, but I also think that we as a tracer–modelling community need to gain more experience in such areas. It is by such concerns that we may improve our sampling strategies in the future.

J. Shepherd. There is no doubt that the limitations of the data are an important factor. Anyone trying to interpret tracer distributions must be tempted to ask for full three-dimensional fields of everything on a one-degree spacing (synoptically), which is obviously not feasible and probably not necessary either. Thus the problem is to make the best possible use of data which are (or may become) available. I would argue that one needs to exercise more care over methodology when working with imperfect data, not less. An important aspect of this is allowing for the known imperfections of the data (for example, the existence of errors), which is why fitting techniques (including inverse methods) are such an appropriate tool. But better data will always help.

C. Wunsch (*Massachusetts Institute of Technology, Massachusetts, U.S.A.*). There are many things to be said (too extensive for this space) about this paper, but perhaps a brief record is possible. It is difficult to understand Dr Shepherd's pessimism. The number of people who have seriously tried to apply inverse methods to tracer data can be counted on the fingers of two hands, if not one. I note that ocean modellers have spent 35 years struggling with forward problems, and all the issues of stability, accuracy, boundary conditions, affordability, etc. Inverse modelling will almost surely require a similar effort, as no one has ever claimed that it was any simpler than for forward problems. Life is hard.

It is worth noting that there are many inverse methods and the most appropriate one to use depends upon the question being asked, the context, convenience, etc. In particular, there is no reason at all why the parameters found through an inverse calculation cannot be required to reproduce the data in the corresponding forward computation. But like any powerful tool, inverse methods can be dangerous to both the user and onlooker. One does not condemn automobiles as useless because they are capable of damage both to driver and bystander.

The intrinsic nonlinearity of most oceanographic inverse problems has been apparent from the beginning. But I would argue that the concentration on linearized versions has been the only reasonable approach in the learning process. The insights gained from linear problems are surely a necessary first step toward ultimate solution of the nonlinear ones. It was known in the nineteenth century that the Navier–Stokes equations are also intrinsically nonlinear. Would one argue that recognition of this nonlinearity should have prevented generations of fluid dynamicists from attempting to first solve linear problems?

J. Shepherd. It is true that the total effort on applying inverse methods has been quite modest. It is still disappointing that a technique that seems so apt turns out to be a little trickier than we thought, but I agree that it is much too soon to become discouraged.

I also agree that the inverse methodology is very powerful but deceptively difficult to drive. Its main virtue is, I think, that, properly applied, it forces one to face up to indeterminacies, the features of the solution that are not determined by the data. Extracting and understanding this information is not always easy, but invariably instructive. The danger with more subjective methods is that one can continue to delude oneself about what is determined and what is not.

The nonlinearity of the problem may have been apparent to Professor Wunsch and his colleagues from the start, but it has not received so much attention as the linear problem and I suspect that it has not been as widely appreciated as it deserves. It is quite possible that the linear methods are giving us most of the answer, and that the main problems lie elsewhere (for example, with the data, or structural indeterminacies, or problems of spatial scale, or box structure). Even so, I would expect everyone to agree that sooner or later we have to allow for errors in the data in a systematic way, and that means that we should not forget about the nonlinear problem even if it is expedient to work for the present with linear systems. Furthermore, if we can find efficient ways to solve the nonlinear problem, it may be desirable to use them, to avoid possible side effects or interactions with other problems.

J.-F. Minster (*CNES/GRGS, Toulouse, France*). The total inversion technique was used in the paper by Wunsch & Minster (1982) because it was recognized that the coefficients of the matrix were affected by errors and because the 'unknown' parameters cannot, in fact, take any value. The method is certainly useful. It suffers from two difficulties: it is computationally heavy (although this is becoming a less severe problem as the machine capacities are improving) and it is nonlinear. As a consequence, there are possibly several minima to the minimization function, and the solution tends to stay close to the *a priori* estimates. These *a priori* values and their errors have thus to be solved very carefully.

J. Shepherd. It does seem to me that the total inversion method is rather a sledgehammer approach to the problem, and I would personally be happier if we could find a scalpel or even a knife that would do the job. In addition, I find those methods that only compute departures from an earlier solution unappealing. Strong dependence on a prior solution implies serious (and maybe structural) indeterminacy in the problem, which should be investigated and pinned down somehow. I am glad to hear that work with total inversion methods is proceeding but I do not think I would encourage the young and innocent to get involved with it.

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