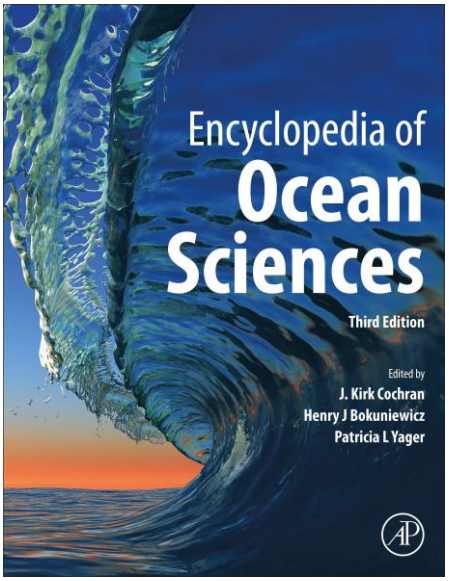

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Inverse Problems, Inverse Methods, and Inverse Models☆

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Introduction

"Inverse methods," "inverse problems," "inverse models" are amorphous overlapping labels for a wide variety of problems and solutions in many different contexts, but ones that commonly arise with the use of observations. In oceanography, as in most sciences, problems involving real observations are *always* "ill-posed" in one or more senses: Data are inevitably noisy, meaning that at best, problem solutions are never unique. They may be too few to solve for some desired quantity, even were they perfect. Data may also be contradictory, and may be all of these things at once: inadequate, and contradictory. But unless observations are just irrelevant to the problem under consideration, inadequate and contradictory data can still contain a bounty of useful information.

In mathematical subjects, inverse problems are commonly defined as "inverse" to a conventional, well-posed, "forward" or "direct" problem. A famous example was discussed by Kač (1966): "Can you hear the shape of a drum?" The forward problem is a conventional one from mathematical physics: given a two-dimensional membrane with a known boundary and physical properties, to calculate the normal mode frequencies. For nonpathological properties, the forward solution is uniquely defined with mathematically desirable properties such as a continuous dependence on the physical parameters. It is "well-posed." The *inverse* problem is: given *all* the normal mode frequencies, to determine the shape of the drum. Years later, it was proven that the answer was not unique, even with the infinite number of normal mode frequencies known perfectly (Gordon and Webb, 1996; Sabatier, 2000).

Problems such as that of Kač have generated a substantial mathematical literature. That literature often assumes an infinite number of perfect "data" are available. A much more practical version of the same problem is: Given a *finite* number of *approximately* known measured normal mode frequencies, and a governing equation with *approximately* known physical parameters, estimate the shape of the boundary, determine also the reliability of the solution, and which of the frequencies are most important to the results. A plausible first-guess at the boundary shape would usually be available, possibly with some understanding of how far it might deviate from the correct one. Or perhaps the boundary is already approximately known, and the information is to be used instead to find a better value for the physical parameters. (A closely analogous problem is that of determining Earth parameters from the measured free oscillation frequencies.)

A very large mathematical literature exists concerning existence, continuity, uniqueness, etc. of the solutions to the mathematicians' inverse problems of various sorts. While very interesting (e.g., Lions, 1971 and several more recent books; and numerous papers in the journal *Inverse Problems* and elsewhere), many of these results are irrelevant to what might be called "inverse problems in practice." Notice that Kač's problem, and its solution, do not involve any form of statistical inference—whereas in practice, inverse problems involving data inevitably do so. One might distinguish mathematical inverse problems from practical ones by noticing that the latter are almost universally forms of statistical estimation problems.

An oceanographic definition of a practical inverse problem is one that involves making inferences from real data (finite in number, inaccurate, possibly contradictory) in the context of one or more equations representing physics, chemistry, dynamics, or biological processes etc., or all at once. Methodologies have been reinvented and relabeled in very diverse fields, and encompass much of general statistical estimation theory in all its forms (frequentist, Bayesian) as well as the understanding and construction of physical models of arbitrarily large dimension and complexity. Because of the reinvention and the possibly willful suppression of common terminologies, competing jargons represent a serious communication problem. Most practical inverse problems are, however, readily unified as subelements of *control theory* in both its engineering and purely mathematical manifestations.

☆*Change History*: May 2018. Carl Wunsch completely rewritten this article.

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Inverse problems in geophysics and oceanography do have a very long history although the recent terminologies and methods depend directly upon the availability of massive computer power. An outstanding early example is the well-known problem of determining Earth's interior mass distribution from measurements of the surface gravity field on both land and at sea. Also ancient is the problem of determining the interior Earth magnetic field from surface data alone.

Although the origins of these problems lies deep in the history of physics and mathematics, to the time of Newton, Laplace, Legendre, Gauss, etc., a convenient discussion starting point was the formulation by A. N. Kolmogorov and N. Wiener of the prediction problem for linear systems (Kolmogorov, 1939; Wiener, 1942, 1949; see Robinson, 1959; Yaglom, 1962). A distinction was made between the problem of predicting the behavior of a system (in Wiener's case, aircraft dynamics—for fire control of anti-aircraft guns), and the "smoothing" problem which corresponds to determining instead the physics of an aircraft from observations of its movement and some knowledge of its dynamics. Statistical inference was combined with a knowledge of dynamics. Wiener employed the covariance of noise and signal for statistically stationary systems in his formulation of the prediction problem. Later, Kalman (1960) inserted a specific time-evolving model of the physics. But because a stationary (In this context, the term "stationary" always means statistically steady and does *not* mean a nonmoving system.) linear system is completely described by its covariance, a specification of the dynamical evolution was already contained in Wiener's theory.

In the geophysical context, the papers beginning with Backus and Gilbert (1967, 1968), (and see particularly Parker, 1994), who introduced the "inverse" problem terminology. Their focus was on geophysical problems including marine data, particularly seismic wave ones, with the goal of determining the static Earth properties through which propagation took place. They used a formalism of continuous space and time, rendering the problems part of the mathematics of functional analysis. They introduced the requirement that useful inverse methods should be able to cope with "inadequate, inaccurate, and contradictory" data (Backus, 1970), and should produce estimates of which solution elements were determined ("resolving power"), which were accurately determined ("variance"), and which of the data were most useful.

So many different estimation problems exist across the oceanographic sciences that lumping them into the "inverse" problem basket is not obviously very helpful, except to note their mathematical commonality. Thus "data assimilation," originating in numerical weather forecasting, is an approximate form of the Wiener-Kalman prediction solution and is part of predictive control theory; "state estimation" is the "smoothing" problem of control theory; "objective mapping" or "objective analysis" and "3dVAR" are forms of weighted least-squares and rely upon the Gauss-Markov minimum variance estimators; "4dVAR" and the "adjoint optimization" are the method of Lagrange multipliers. As with many problems in science, a focus on mathematical methods or particularities of numerical algorithms can obscure the more fundamental issues: formulating the problems using all available insights into the physics, chemistry, biology, or geophysics as well as the detailed knowledge of how, where, and with what accuracy observations were obtained and what accuracy is required in the solution elements.

Specific Example

To define terms, consider a classical problem of elementary physics and calculus, that of a damped oscillator written as,

$$M\frac{d^2x(t)}{dt^2} - r\frac{dx(t)}{dt} + kx(t) = q(t),$$
$$x(0) = x_0,\ \frac{dx(0)}{dt} = x'(0),\ t \geq 0. \tag{1}$$

Here M, r, k are all fixed numbers, and $q(t)$ is a known function. With the initial conditions at $t = 0$ as provided, this example is a much studied well-posed *forward* problem: the solution is (1) unique, (2) continuous, (3) differentiable (Thinking of t as time is useful, but in practice, it can be any independent variable or index that locates x.). Conventional mathematics and physics textbooks instruct the reader that only such "well-posed" problems should be undertaken.

If the problem is stated in only slightly different ways however, the question of wellposedness has to be considered again. For example,

(A) Suppose $x(t)$ is known, but M and/or r, and/or k are to be determined.
(B) The initial condition, x_0, is not perfectly known, but is described for example, as $x_0 \pm \Delta x_0$ where Δx_0 is some indication of uncertainty in the value of x_0.
(C) None of the initial conditions are known, but instead $x(t_1)$, $x(t_2)$, $x(t_3)$, ... are provided. Can one still determine $x(t)$? Suppose these values are only imperfectly determined?
(D) $x(t)$ is known for all times, $t > 0$. Can $q(t)$ be found? Suppose $x(t)$ is imperfectly known?
(E) ....

In general, all of these variant problems are ill-posed. For example, (B) renders the solution nonunique. (C), even with perfect measurements, potentially has too much information unless the known values satisfy special constraints. In (D), if $x(t)$ and all the parameters are known, $q(t)$ is fully-determined, unique, differentiable etc. If $x(t)$ is imperfectly known, then $q(t)$ is no longer unique

and perhaps not continuous or differentiable. Problem (D) is plainly a control problem—finding which forces acting would have produced the observed trajectory, $x(t)$?

In some of these cases, special "inverse methods" are required. In other cases, for example, (D) with perfectly known $x(t)$, simple differentiation suffices. In all cases (A–D), the Eq. (1) has become an "inverse model". Sometimes the correct model is itself unknown and the inverse model may differ, for example, by omission of the term $rdx\,(t)/dt$. Ideally, an inverse model is fully consistent with or identical in structure to an underlying forward model (Some early papers, by authors hostile to the use of oceanographic inverse methods, deliberately used incorrect models and leading them to the erroneous conclusion that the methods failed. Sometimes model inadequacy is not obvious. The famous "abyssal recipes" calculation by Munk (1996) is an inverse problem for oceanic mixing and advection velocities; but the inverse model (a 1-dimensional advection-diffusion equation) has come, decades later, to be regarded as inapplicable (e.g., Ferrari et al., 2016). So-called robust control theory includes methods for dealing with classes of models, rather than specific ones.).

In a time of fast, cheap, digital computers, almost all such problems are, in practice, solved numerically. So for example, Eq. (1) can be discretized in a number of different ways. (As early as Levinson 1947a, b, it was clearly recognized that discretization of the Wiener-Kolmogoroff theory rendered the mathematics simply a form of least-squares. That made it accessible to a wide application community that had struggled with the continuous time theory.) The simplest is an ordinary backward difference at equal time steps Δt,

$$\frac{M}{\Delta t^2}\left[x((n+1)\Delta t) - 2x(n,\Delta,t) + x((n-1)\Delta t)\right]\frac{r}{\Delta t}\left[x(n,\Delta,t) - x((n-1)\Delta t)\right] + kx(n,\Delta,t) = q(n,\Delta,t), \tag{2a}$$

$$n = 0, 1, 2, \ldots, \quad x(0\Delta t) = x_0, \quad (x(\Delta t) - x(0\Delta t)) = \dot{x_0}(\Delta t), \tag{2b}$$

and which is readily rearranged, in matrix-vector notation (this article assumes familiarity with basic matrix-vector notation. In general, bold upper case letters are matrices, bold lower case letters are column vectors. Superscript T implies transposition so that e.g., $\mathbf{x}(t)^T$ is a row vector. Superscript -1 denotes an ordinary matrix inverse. Some elementary statistical notions are used, including that of the bracket $\langle . \rangle$ to denote a true (hypothetical) average.), as,

$$\begin{aligned} &\mathbf{A}\mathbf{x}(n,\Delta,t) = \mathbf{q}(n,\Delta,t), \text{ or} \\ &\mathbf{A}\mathbf{x}_a = \mathbf{q}_a, \end{aligned} \tag{3}$$

$$\mathbf{x}_a = \left[\mathbf{x}(0\Delta t)^T, \mathbf{x}(1\Delta t)^T, \ldots\right]^T, \mathbf{q}_a = \left[\mathbf{q}(0\Delta t)^T, \mathbf{q}(1\Delta t)^T, \ldots\right]^T$$
$$\mathbf{A} = \begin{Bmatrix} 2 - \frac{r}{M}\Delta t - \frac{k}{N}\Delta t^2 & \frac{r}{\Delta t} - 1 \\ 1 & 0 \end{Bmatrix} \tag{4}$$

where $\mathbf{x}_a$, $\mathbf{q}_a$ represent a stacking into one column vector of the entirety of all of the time-dependent elements of the vectors $\mathbf{x}\,(t)$, $\mathbf{q}\,(t)$. The stacked system, Eq. (3), is a collection of simultaneous equations whose solution is *the* unique solution to the classical forward problem. An equation count shows an equal number of unknowns, N, and of equations, and thus the solution can be written,

$$\mathbf{x}_a = \mathbf{A}^{-1}\mathbf{q}_a. \tag{5}$$

With the classical initial conditions in Eq. (2b), the $N \times N$ matrix inverse $\mathbf{A}^{-1}$ exists. On the other hand, solving the set through multiplication by $\mathbf{A}^{-1}$ is a procedure unlikely to be adopted—because an even better approach is by time-stepping: solve the first equation for $\mathbf{x}\,(\Delta t)$, and use it to find $\mathbf{x}\,(2\Delta t)$, etc. This method is fast and easy, and is probably the same solution is in Eq. (5). Note however, that if for example, $\dot{\mathbf{x}_0}(\Delta t)$ is missing, but $\mathbf{x}(t_q)$,any $t_q \neq 0$, is known instead, sufficient information still exists to solve the resulting simultaneous equations uniquely and stably; but ordinary time-stepping no longer works because the starting conditions are not fully known. Eq. (3) remains correct and useful, and its wholly generic form reinforces the possibility that t is an arbitrary accounting index, neither necessarily time nor uniformly spaced.

A basic understanding of practical inverse problems and their solutions can generally be reduced to the recognition that they are *always* equivalent to sets of simultaneous algebraic equations, both linear and nonlinear, with more than, fewer than, or equal numbers of equations than unknowns. To avoid matrix inversions, advantage is often taken of the particular structure of the simultaneous equations as in the time-stepping. But generally, any useful solution method will at least approximate that found by Eq. (5) or its extensions to nonlinear systems.

Now suppose the problem is rendered a bit more realistic by assuming that the forcing $\mathbf{q}\,(t)$ came from measurements, and thus includes "noise," so that it is replaced by $\mathbf{q}(t) = \mathbf{y}(t) - \mathbf{n}(t)$ where $\mathbf{n}(t)$ is a noise field, often with known mean and statistical second moments $\langle \mathbf{n}(t)\mathbf{n}(t)^T \rangle = \mathbf{R}(t)$. t remains a discrete independent variable, and which has the great advantage of side-stepping the major complexities of the mathematics of continuous-time stochastic processes and partial-differential equations (e.g., Gardiner, 2004). For convenience, it will be assumed that the mean $\langle \mathbf{n}(t) \rangle = \mathbf{0}$ and which can usually be arranged with adequate accuracy. The minus sign introduced in front of $\mathbf{n}(t)$ is placed there only so that Eq. (3) is re-written conventionally as,

$$\mathbf{A}\mathbf{x}_a + \mathbf{n}_a = \mathbf{y}_a, \tag{6}$$

all vectors being "stacked." Supposing for the moment that $\mathbf{A}$ is unchanged from before—how to proceed? One approach is to replace $\mathbf{n}_a$ by its average value of zero, writing

$$\tilde{\mathbf{x}}_a = \mathbf{A}^{-1}\mathbf{y}_a,$$

where the tilde has been used to distinguish this solution from that in Eq. (5) and noting that it is not necessarily the only solution.

Is this a *useful* solution? Note that,

$$\tilde{\mathbf{x}}_a = \mathbf{A}^{-1}\mathbf{y}_a = \mathbf{A}^{-1}(\mathbf{q}_a - \mathbf{n}),$$

and its difference from the hypothetical correct solution, $\mathbf{x}_a$, is

$$\tilde{\mathbf{x}}_a - \mathbf{x}_a = -\mathbf{A}^{-1}\mathbf{n}_a,$$

whose mean (expected value) is zero, $\langle \tilde{\mathbf{x}}_a - \mathbf{x}_a \rangle = 0$, so it is *unbiassed*. On the other hand, its second moments are,

$$\left\langle (\tilde{\mathbf{x}}_a - \mathbf{x}_a)(\tilde{\mathbf{x}}_a - \mathbf{x}_a)^T \right\rangle = \mathbf{A}^{-1}\langle \mathbf{n}_a \mathbf{n}_a^T \rangle \mathbf{A}^{-T} = \mathbf{A}^{-1}\mathbf{R}\mathbf{A}^{-T},$$

and which, depending upon both the structure and magnitudes of $\mathbf{A}$ and $\mathbf{R}$, may have diagonal values (the variances of the solution elements about the correct value) that are acceptably sized, or unacceptably large or small. Notice that while a perhaps useful solution has been found, no further information concerning $\mathbf{n}(t)$ has emerged and if the solution proves unacceptable, what to do next?

Now add a bit of information in the form of *measurements* at a few times, t_j, of the solution vector $\mathbf{x}(t_j)$ or of the velocities, $[\mathbf{x}(t_j) - \mathbf{x}(t_{j-1})]/\Delta t$, or conceivably even accelerations or other combinations. Seeking realism, these all contain some form of error, $\varepsilon(t_j)$, again assumed to be of zero mean, and known second moments. Let all of these extra pieces of information be written as another set of simultaneous equations,

$$\mathbf{B}\mathbf{x}_a + \varepsilon_a = \mathbf{p},$$
$$\varepsilon_a = \left[\varepsilon(t_1)^T, \varepsilon(t_2)^T, \ldots\right]^T$$

for all those times when an observation is available. $\mathbf{B}$ might be very sparse, with few rows, picking out only those elements for which an observation is available. Suppose there are P values of such noisy observations. The rows of the usually sparse $P \times N$ matrix $\mathbf{B}$ will consist of either a single element of 1 and all the rest zeros (if $x(t_j)$ is measured, or 1 and -1 and all zeros, if $\mathbf{x}(t_j) - \mathbf{x}(t_j - 1)$ is measured, etc.).

This new set of simultaneous equations can be combined with the old set, Eq. (6), into the combined form,

$$\mathbf{E}\mathbf{x}_a + \mathbf{n}_a = \mathbf{y}_a,$$

where now $\mathbf{E}$ is $M = (N + P) \times N$. Some of the equations come from observations, and some from relationships amongst them (a "model"). Now there are $N + P$ equations in N unknowns $\mathbf{x}_a$ and the equation set now appears to be *over-determined*. Over-determined sets of algebraic equations are very familiar, and one learns in elementary calculus to find the solution $\tilde{\mathbf{x}}_a$ that makes the magnitude of $\mathbf{n}_a$, measured as $\mathbf{n}_a^T\mathbf{n}_a$, a minimum. A formal, and readily generalizable, result is through ordinary least squares. Form an objective or cost function, J, such that

$$J_1 = (\mathbf{y}_a - \mathbf{E}\mathbf{x}_a)^T(\mathbf{y}_a - \mathbf{E}\mathbf{x}_a) = \sum_i \mathrm{n}_{ai}^2.$$

Taking the partial derivatives of J with respect to $\mathbf{x}_a$ leads immediately to,

$$\tilde{\mathbf{x}}_a = (\mathbf{E}^T\mathbf{E})^{-1}\mathbf{E}^T\mathbf{y}_a.$$

Some inference now can be made about $\mathbf{n}$ as well:

$$\tilde{\mathbf{n}}_a = \mathbf{y}_a - \mathbf{E}\tilde{\mathbf{x}}_a = \mathbf{y}_a - \mathbf{E}(\mathbf{E}^T\mathbf{E})^{-1}\mathbf{E}^T\mathbf{y}_a.$$

Notice that information about the second moments, $\mathbf{R}$, has not been used. Also, the rationale for choosing the smallest magnitude $\mathbf{n}_a$ solution is not obvious. Even so, $N + P$ solution elements appear to have been determined (N of them for $\mathbf{x}(t)$, and P of them for $\mathbf{n}(t)$) and the claim of "over-determination" looks fragile. Note too, that any change in the estimated noise, $\tilde{\mathbf{n}}(t)$, leads immediately to a change in $\tilde{\mathbf{x}}(t)$. Unless the noise were actually known a priori, this solution can hardly be regarded as more than a purely ad hoc one.

Employment of knowledge of $\mathbf{R}$, and often of some knowledge of the second moment matrix of $\mathbf{x}(t)$, leads to generalizations of the least-squares solution to account for that information. Again, a simple approach is through least squares, minimizing,

$$J_2 = (\mathbf{y}_a - \mathbf{E}\mathbf{x}_a)^T\mathbf{R}^{-1}(\mathbf{y}_a - \mathbf{E}\mathbf{x}_a) + \mathbf{x}_a^T\mathbf{S}^{-1}\mathbf{x}_a. \quad (7)$$

For these general methods the reader is referred to extended discussions in Lawson and Hanson (1995), Menke (1989), and Wunsch (2006a, hereafter W06) and many other textbooks. Statistics enter immediately in tests of whether the resulting solution from minimizing J_2 is consistent with the prior estimates of the noise and solution covariances $\mathbf{R}$, $\mathbf{S}$.

In many cases, one of which is described below, the number of equations is less than the number of unknowns, $\mathbf{x}_a$, and *always*, of the combined set $\mathbf{x}_a$, $\mathbf{n}_a$. The message of inverse methods more generally is that whatever the number of equations, they carry information about the solution, and the goal is to determine (A) what aspects of the solutions $\mathbf{x}_a$, $\mathbf{n}_a$ is implied by the equations that do exist, and how well can they be determined? and (B) what are the elements of $\mathbf{x}_a$, $\mathbf{n}_a$ about which no information is available? (C) Can the data be ranked in order of importance to the solution chosen?

Practical inverse problems and methods require a great deal of attention to be paid to the noise elements, their statistics, and consistency with any prior hypotheses—leading to an essentially Bayesian approach and a heavy emphasis on knowledge of physics, or chemistry or biology. Consider one example of an *underdetermined* problem,

$$\mathbf{E}\mathbf{x}_a + \mathbf{n}_a = \mathbf{y}_a \tag{8}$$

where $\mathbf{E}$ is $M \times N$, with $M < N$ that is, it is formally underdetermined in $\mathbf{x}_a$—even should the noise vanish. Some of the equations can again come from observations, and some from known relationships amongst them (a model). *A* solution is, found by arbitrarily minimizing the size of $\mathbf{x}_a$ from

$$J_3 = \mathbf{x}_a^T \mathbf{x}_a$$

which obviously has a minimum of zero and as a complete solution implies that the observations and model relationships are all noise: $\mathbf{n}_a = \mathbf{y}_a$, and is of little interest. An easy way to insist that the minimum length solution also satisfy the equations is to write

$$J_4 = \mathbf{x}_a^T \mathbf{x}_a - 2\boldsymbol{\mu}^T \left(\mathbf{y}_a - \mathbf{E}\mathbf{x}_a\right). \tag{9}$$

(see, W06, P. 58+). Here, $\boldsymbol{\mu}$ is a vector of "Lagrange multipliers" and which is treated as a new set of unknowns. Setting to zero the partial derivatives of J_4 with respect to both $\mathbf{x}_a$, $\boldsymbol{\mu}$, produces.

$$\tilde{\mathbf{x}}_a = \mathbf{E}^T \left(\mathbf{E}\mathbf{E}^T\right)^{-1} \mathbf{y}_a,$$
$$\tilde{\boldsymbol{\mu}} = -\left(\mathbf{E}\mathbf{E}^T\right)^{-1}, \tilde{\mathbf{n}}_a = 0$$

which is the classical underdetermined solution that minimizes the norm $\tilde{\mathbf{x}}_a^T \tilde{\mathbf{x}}_a$ and which might seem to be a sensible choice. On the other hand, $\tilde{\mathbf{n}} = \mathbf{0}$ is an unacceptable solution if the $\mathbf{y}_a$ (or $\mathbf{E}$) contain errors and which thus must lead to rejection of this solution. In Eq. (9), $\mathbf{E}\mathbf{x}_a = \mathbf{y}_a$ appears as a "hard constraint"—that is the equations must be satisfied exactly (forcing $\tilde{\mathbf{n}}_a = \mathbf{0}$). The use of hard constraints has led some authors to claim that they *require* the equations be satisfied exactly. Although that can be true, an obvious and sensible generalization of J_4 is to include an error term in the equations and include minimization of the noise as part of the solution for example, as,

$$J_5 = \mathbf{x}_a^T \mathbf{x}_a - 2\mu^T \left(\mathbf{y}_a - \mathbf{E}\mathbf{x}_a - \mathbf{n}_a\right) + \mathbf{n}_a^T \mathbf{n}_a, \tag{10}$$

probably with corresponding covariance weights as in J_2 (see Eq. 11 below).

A General Least-Squares/Gauss Markov Result

Depending upon investigator knowledge and insights, a great variety of information about the solution and which *always* includes the noise field, can and should be used to formulate the inversion. A very general formalism invokes classical discrete least-squares. Consider a cost or objective function

$$J = \underbrace{\left(\mathbf{y}_a - \mathbf{E}\mathbf{x}_a\right)^T \mathbf{R}^{-1} \left(\mathbf{y}_a - \mathbf{E}\mathbf{x}_a\right)^T}_{\text{noise}} + \underbrace{\left(\mathbf{x}_a - \mathbf{M}\mathbf{x}_0\right)^T \mathbf{S}^{-1} \left(\mathbf{x}_a - \mathbf{M}\mathbf{x}_0\right) - \text{prior values of x}}_{} \underbrace{2\boldsymbol{\mu}^T \mathbf{L}\mathbf{x}_a}_{\text{model constraints}} \tag{11}$$

generalizing Eq. (10) where $\mathbf{R}$ and $\mathbf{S}$ are above, $\mathbf{x}_0$ is an a priori estimate of $\mathbf{x}_a$, and $\boldsymbol{\mu}$ are again Lagrange multipliers (sometimes called the "adjoint solution"). $\mathbf{E}$ relates $\mathbf{x}_a$ to $\mathbf{y}_a$, $\mathbf{M}$ picks out the values or combinations of values in $\mathbf{x}_a$ for which there is prior information, and $\mathbf{L}$ indicates various known relationships between elements of $\mathbf{x}_a$ as might be true in a model, but including any error terms.

To a large extent, many of these different appearing terms can be interchanged. (For example, $x_2 - x_1 = 1 + \varepsilon_1$ can be imposed using a Lagrange multiplier and adding ε_1 to the state vector $\mathbf{x}_a$. Alternatively, it can be regarded as equivalent to an observation of $x_2 - x_1$ with a noise element ε_1 included in $\mathbf{n}_a$. A lot of flexibility is available for convenience purposes.) Additional terms involving for example, internal parameters and their prior values are easily accommodated. As discussed in the textbooks, use of Eq. (11) is equivalent to solving a *weighted* set of simultaneous equations, where the weights are derived from $\mathbf{R}$, $\mathbf{S}$ etc. usually through a Cholesky decomposition. Least-squares is very flexible, including classes of constraints involving inequalities (see W06, P. 164+ for references).

Differentiating J with respect to $\mathbf{x}_a$, and $\boldsymbol{\mu}$ leads to a set of ordinary least-squares "normal equations." For very general numerical approaches to solutions of these equations (which are the same as finding the stationary values of J) (Here "stationary" is used in the

sense of the values of **x**, **n**, μ where the derivatives vanish and should not be confused with "stationary statistics."), the voluminous literature on optimization includes Gill et al. (1986).

An Underdetermined Problem: The Level of No Horizontal Motion

Probably the first explicit application of an inverse method in physical oceanography was directed at the famous problem of determining a "level-of-no-motion" in the oceanic circulation. As classically formulated, the absence of a "level-of-known-horizontal-motion" in the ocean led physical oceanographers to assume that there existed a depth, z_0 (x,y) where the large-scale horizontal flow vanished. Consider a pair of ordinary hydrographic stations, where temperature, T (z, x_i, y_i), and salinity, S (z, x_i, y_i) and hence the density difference, $\Delta\rho$, between them can be calculated as a function of depth. By using the thermal wind relations, at nonequatorial latitudes, the flow normal to the pair can be computed numerically from,

$$\rho f \frac{\partial u_{\perp}(z,x,y)}{\partial z} = g \frac{\partial \rho(z,x,y)}{\partial r}, \tag{12}$$

where $u_{\perp}$ is the flow normal to the pair, and r is the distance between them and which by rendering discrete can be integrated in the vertical so that,

$$u_{\perp}(z,x,y) = \frac{g}{\rho f} \sum \frac{\Delta\rho(z,x,y)}{\Delta r} + u_{0i},$$

where u_0 is an integration constant that arises from the vertical integration in Eq. (12) that starts at some depth z_0 where u_{0i} would be the flow. How to determine u_0? The problem as initially formulated took a closed volume of ocean, surrounded by N-hydrographic station pairs. By demanding that the total transport of fluid flowing in must equal (nearly—within error estimates) the flow outward, one obtains a single equation (constraint) on the N unknown u_{0i}. By writing similar near-conservation rules for mass, salt, oxygen, etc. and for these and other properties in various density layers within the water column, a large number of constraints can be constructed. At the end however, typically fewer equations than unknowns results, and an inverse method must be used to describe the full family of solutions. See Figs. 1 and 2 and W06.

Estimates of uncertainty are one of the most important outcomes of a true inverse procedure.

Light gray line in upper left corner is a mean depth of the Scotia Arc east of Drake Passage.

A number of applications including oxygen and nutrients (e.g., Ganachaud and Wunsch, 2002) have also been published.

Time-Dependent Problems

The ocean is a time-dependent fluid flow, one containing time-dependent chemical and biological fields. That inescapable observational reality leads to the formulation of time-dependent inverse problems. Note that already, Eq. (1) describes a time-dependent state, but its solution was reduced to a set of simultaneous algebraic equations. That the indexing variable was time made no difference: that variable could be replaced by a space or any other bookkeeping index.

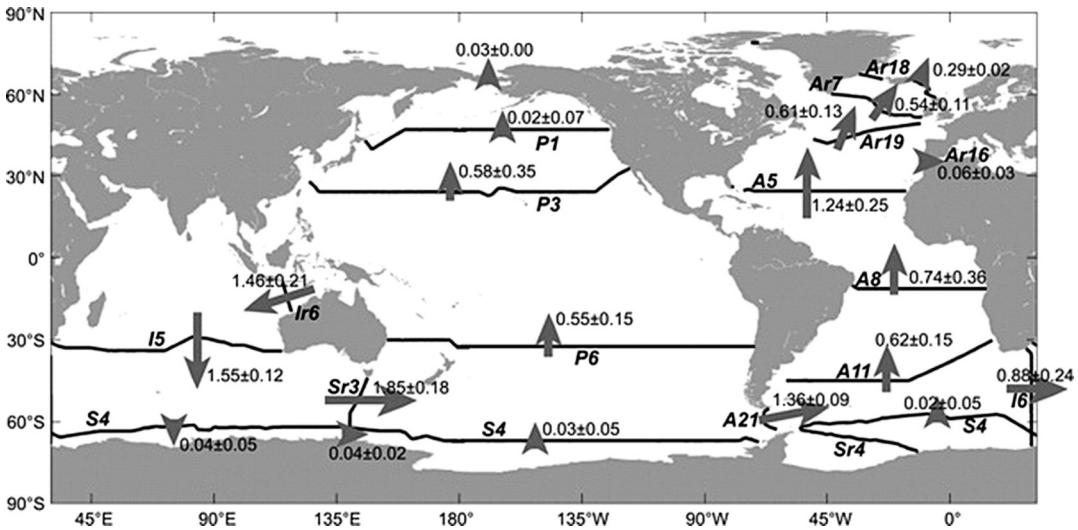

Fig. 1 Example of a static inversion (Lumpkin and Speer, 2007) showing the large-scale boxes used to write approximate (that is, noisy) balances for determining the unknown reference levels.

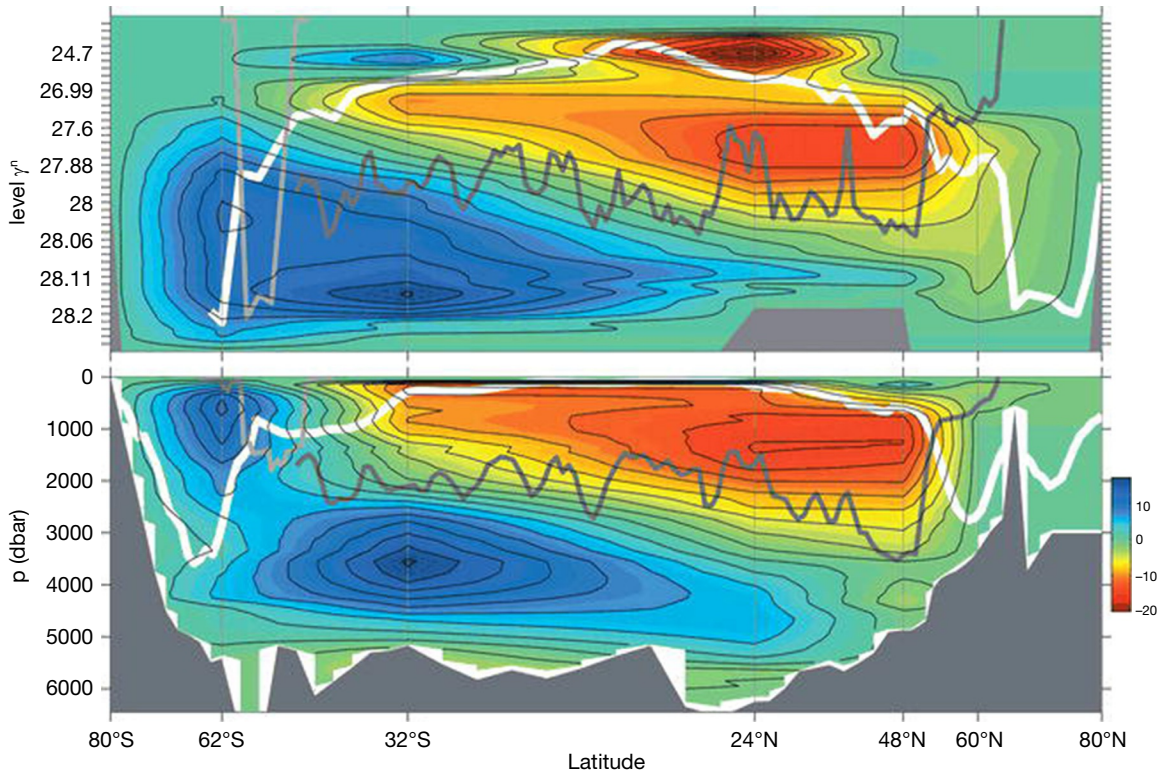

Fig. 2 Solution to underdetermined static flow inverse problem by Lumpkin and Speer (2007) showing the zonally integrated global stream function (Cf. Ganachaud, 2003). *Gray line* indicates mean mid-ocean ridge crest height. *Thick white line* represents the zonal mean mixed layer depths.

The major issue is that time-dependent problems in real fluids like the ocean generate enormous volumes of describing numbers—via partial differential equations, and even though such problems can once again in principle be reduced to sets of simultaneous equations, linear and nonlinear, the dimensionality requires various "tricks" to cope. Most of those tricks however, can be regarded as clever ways of approximately solving the simultaneous equations without having to store them all at once in the computer—even though the solutions are equivalent—if properly carried out.

Consider the equations of fluid- and thermo-dynamics, and of chemistry and biology as written on a computer. Again a "state vector," $\mathbf{x}(t)$, exists, often of enormous dimension (39×10^6 at one time, t in one example; such a model, time-stepped hourly for 20 years would generate an equivalent $\mathbf{x}_a$ of dimension $N = 7 \times 10^{12}$ elements; Forget et al., 2015). A computer model of $\mathbf{x}(t)$ is a time-stepping rule,

$$\mathbf{x}(m\Delta t + \Delta t) = \mathbf{L}(\mathbf{x}(m, \Delta, t), \mathbf{p}, \mathbf{q}(t)), \tag{13}$$

plus a set of initial conditions, $\mathbf{x}(0)$, $\mathbf{x}'(0)$, and boundary conditions, $\mathbf{x}(\mathbf{r},t) = \mathbf{x}_B(\mathbf{r}_B,t)$. Typically, the elements in any $\mathbf{x}(m\Delta t)$ are three component velocities, (u, v, w), temperatures T, salinities S and a pressure, p, at every grid point or finite element of a computer code. The time-stepping operator, $\mathbf{L}$, is the computer code, comprised of hundreds of thousands or even millions of lines. $\mathbf{q}(t)$ can contain external boundary conditions (e.g., momentum and thermodynamic exchanges with the atmosphere) as well as any kind of interior forcing, sources and sinks (if e.g., the model contains decaying radiocarbon). $\mathbf{p}$ denotes any interior model parameters including mixing coefficients, bottom topography, et al.

Construction of such forward computer model codes that lead to accurate, stable, solutions $\mathbf{x}(t)$ is a highly developed, sophisticated, subject with roots extending back to about 1950. These models typically are time-stepped from their initial conditions subject to spatial/−temporal boundary conditions and forcing. A good code will be in terms of algorithms producing well-behaved solutions in terms of required accuracy, precision, etc. and might even display numerical convergence to the underlying hydrodynamic/thermodynamic equations (although rarely demonstrated). Resulting equations are numerically well-posed.

Eq. (13) in theory could again be written out as a set of stacked coupled, perhaps nonlinear equations, and solved in theory by various computer algorithms that ignore the very special structure that permits a time-stepping solution. Notice that just as with the simpler Eq. (1), the stacked problem can be rendered numerically ill-posed in the same large-number of ways: uncertainties in initial conditions and boundary conditions, in the interior parameters, $\mathbf{p}$, the provision of noisy observations, etc. When any or all of these conditions is present, the system is ill-conditioned and is best treated as an inverse problem. The huge dimensions possible

has led to an equally huge, sometimes highly technical, literature directed at the computer methods necessary to cope—without directly solving the stacked system. One example is Utke et al. (2008).

Time-dependence too, brings a focus onto prediction capabilities. (Spatial extrapolation is a problem in exploration geophysics for locating ore bodies, and are closely analogous. See Armstrong (1989) for the specialized methods used there.) In particular, the problems of weather forecasting have led to an entire subject labeled "data assimilation" with a whole series of specialized methods and terminologies specific to the prediction problem—an outgrowth of the Wiener-Kolmogoroff theories alluded to above.

Precisely the same objective function J as in Eq. (11) can be used. If prediction is the goal, a term, perhaps with a heavy relative weight, corresponding to,

$$(\tilde{\mathbf{x}}(t_{\text{future}}) - \mathbf{x}(t_{\text{future}}))^T \mathbf{S}_{\text{future}}^{-1} (\tilde{\mathbf{x}}(t_{\text{future}}) - \mathbf{x}(t_{\text{future}})),$$

can be added, where t_{future} is the prediction time. The weight matrix, $\mathbf{S}_{\text{future}}^{-1}$, could be so large that all other terms in the objective function J are negligible, giving priority to an accurate forecast instead of fitting data at earlier times. The specialized structure of time-stepping models (Eq. 13) permits the use of clever schemes to minimize storage requirements, obtaining solutions by iteration, etc. At the end of it all, however, these schemes produce a solution to the underlying sets of weighted simultaneous equations. If the model, or the observations, are nonlinear in $\mathbf{x}(t)$, iterative solutions are required, but the goal is the same: solve the simultaneous equations as accurately and efficiently as possible. Numerical difficulties can arise; see for example, Gebbie and Hsieh (2017) and the references there.

Prediction Versus Smoothing

At least as far back as Wiener (1942), it was recognized that the problems of forecasting led to different methods than the problems of estimation and understanding. Wiener's theory was directed at the handling of stationary time series, that is ones whose signal and noise statistics were independent of time (and/or space). Given (in theory), the infinite past of a scalar time series, $x(t)$ (and time was continuous in Wiener's theory) until the present time t_{now}, the prediction problem consists of estimating the best predictive value $x(t_{\text{future}} = t_{\text{now}} + \tau)$, $\tau > 0$, and its uncertainty. The "smoothing" problem is directed at $\tau < 0$ so that some formally future values are available for making the estimate, and with that added information a smaller uncertainties are expected at all times $t < t_{\text{now}}$. Because of its use of continuous time and frequency domain methods, Wiener's prediction results involved spectral factorization (a Wiener-Hopf problem) and proved mathematically inaccessible to many users. Levinson (1947a,b) produced a solution to the discrete problem that was a form of least-squares and thus much more useful to a wider community. His solution included extremely rapid recursion methods that were very important in the days of slow and small computers (see Claerbout, 1976).

Kalman (1960) extended the discrete version of the Kolmogoroff-Wiener prediction theory to the nonstationary case, with particular applicability to problems involving a dynamically constrained state. *Transients* such as those involved in missile launch were accounted for, and prediction of impact points and time were the immediate focus. Unlike the Wiener prediction filter for statistically stationary processes, the Kalman prediction filter necessarily involves calculating a time-evolving set of covariance matrices, which, for nonstationary systems change under both the dynamical model and the incoming observational data stream. With modern computers, covariance matrices of square dimension of $N > 1000$ are feasible. With geophysical fluids however, having $N > 10^6$, computation of such matrices is not possible (they require running the model an extra N times at each time-step), and they are held fixed. Thus despite claims to the contrary, published applications are of an extended discrete Wiener theory—the extension being the insertion of a dynamical model to propagate the state vector, but without changing the covariance matrices. When the dynamical model is a nonlinear one, and not linearizable, the statistical assumptions are often ad hoc and not readily testable.

Extensions, Complications

In practice, most inverse problems, whether for prediction or smoothing, are solved as some form of approximate least-squares. Least-squares methods have a strong connection to fields having Gaussian, or at least unimodal, probability distributions. Thus one form of failure can be encountered when distributions of solutions or data errors are multimodal or highly nonGaussian in a variety of ways. So-called robust methods exist, in a variety of forms including changes in the measure of misfit or size from weighted sums of squares $\sum a_i q_i^2$ (2-norm) to different measures, such as the 1-norm, $\sum |a_i q_i|$, or an infinity norm, $\max(|a_i q_i|)$ and these approaches have much to recommend them. 1-norm methods are highly developed in the context of linear programming and are widely used in business applications. Robust methods commonly involve these other norms (See, for example, Yedavalli, 2014).

For very large problems, such as those encountered in oceanic problems, the requirements of computational and storage efficiency demand close attention to computer architectures and details such as input/output requirements. At present, the software available for large-scale ocean problems is much more highly developed for the 2-norm methods than for any of the others.

Because application of time-evolving uncertainty estimates in the standard forms such as the Kalman filter for prediction, or various smoothing methods (see Anderson and Moore, 1979) and sometimes the presence of strong nonlinearities remain computationally beyond reach, resort has been made to Monte Carlo/ensemble methods. Typically (see Evensen, 2009; Kalnay, 2003),

for the weather prediction problem) ensembles of solutions are generated by randomly perturbing initial conditions according to some hypothesized probability density of the errors. Sometimes the fastest growing disturbances can be identified as the generator of major uncertainties in short-range forecasts.

These methods are essential and are likely to remain so for purposes of understanding the degree to which the models produce accurate forecasts. In practice, however, and of particular concern for oceanic problems with their often enormous time scales, the ensemble sizes remain a minute fraction of the number of statistical degrees of freedom in the state. Covariances calculated from the ensemble members will be highly singular, with no representation of uncertainties in most elements of interest. True knowledge of the probability densities of the stochastic elements of the system is another major problem that will need to be solved in the future.

Oceanographic Applications

Static Problems

Many different applications of these principals have been made in the wider oceanographic context. The apparent earliest use for fluid flow was for the assumed static geostrophic box inverse problems described above, and summarized in W06. Amongst numerous later examples are Roemmich et al. (2001), Macdonald (1998), Ganachaud (2003), and Lumpkin and Speer (2007). Biological/chemical examples are Ganachaud and Wunsch (2002) and Macdonald et al. (2003). Extensions of the static problem methods have been discussed at length by Killworth (1986) and Chu (2006), and others.

Marine geodetic and geomagnetic inverse problems have recently been discussed by Mitrovica and Forte (2004) and Korte and Constable (2008), respectively although on the global scale, the distinction between "ocean" and "terrestrial" problems is mainly one of data types and accuracies and not of the physics.

Time-Dependent Problems

Geomagnetic time-dependent problems involving marine data are very important. The secular variation of the geomagnetic field has been of long-standing interest and a recent discussion is in Jackson et al. (2000).

In physical, chemical, and biogeochemical oceanography, as the picture of a static ocean assumption became untenable, attention turned to time-dependent ocean problems. Because of the highly-evolved numerical weather forecast systems, attractively labeled "data assimilation," much oceanic activity simply adopted those methodologies (e.g., Carton and Giese, 2008). That approach conveniently ignored the well-known and long-standing distinction between the goal of a best-prediction, and that of a best-smoothed estimate.

Oceanic problems where prediction is indeed the goal are common, involving particularly forecast of balanced eddy fields (e.g., Hurlburt et al., 2009), military acoustic propagation, and in coupled problems such as El Niño prediction (Sarachik and Cane, 2010). For these problems, the meteorological prediction experience is highly useful.

"Reanalyses"

In an effort to produce useful estimates of the climate system over long periods of time, the meteorological community has used weather models and forecast methods to produce what have come to be known as "reanalyses." (They are reanalyses of the original weather forecasts, but over much longer time spans.) What has been noted repeatedly however, is that for purposes of understanding of the ocean, as opposed to its prediction, smoothing or "state estimation" methods are required to find estimates that obey basic conservation rules for energy, momentum, enthalpy, fresh-water, etc. (see e.g., Fukumori, 2001; Wunsch and Heimbach, 2013).

Useful forecasting is fundamentally an engineering problem and for operational purposes, be it ship routing or acoustic forecasting, failure of a model to be for example, energy or water conserving, is of little or no concern. It only becomes a concern when the results, as in meteorological "reanalyses," are analyzed over climate time-scales for understanding of oceanic and global heat budgets amongst other problems (see e.g., Bengtsson, et al. 2004; Wunsch and Heimbach, 2013).

State Estimation

With the advent of the World Ocean Circulation Experiment (WOCE) in the early 1990s, and the first availability of true nearly-global data sets, oceanographic attention began to turn to the smoothing problem, as the only viable route to understanding of the ocean in climate. Because ocean time-scales are long, even were large-scale ocean circulation forecasts to be attempted, many decades would have to pass before a true test of forecast skill would be possible. In any event, an ultimate goal of ocean climate prediction can only be approached with a better understanding of the physics of today and the recent past. The major example of the smoothing activity is contained in the Estimating the Circulation and Climate of the Ocean (ECCO) program (see Fukumori et al., 2017; Forget et al. 2015) and which solves the multidecadal smoothing problem iteratively, relying upon Lagrange multipliers to both enforce model physics and as a numerical algorithm for minimizing a model-data misfit. Verdy and Mazloff (2017) extended the physical models to biogeochemical ones.

Tomographic problems, whether medical, biological, atmospheric, or oceanographic are by their very nature always inverse problems; see Khil'ko et al. (1998); Munk et al. (1995). Applications of these methods, in various forms, to paleoclimate problems, where the data are "proxies" for physical variables have been discussed by Amrhein et al. (2015), Gebbie et al. (2016), Kurahashi-Nakamura et al. (2017), and Amrhein et al. (2018) amongst others.

The major present problem with all such estimates, as with the results from *any* climate scale model whether data are used directly or not, is in determining the accuracies of various results. For modest sized problems (state vectors of dimensions, N, of a few thousands at any time), the linearized standard methods of filters and smoothers as described in textbooks work well. But with the very large state vectors of global ocean problems, the computational burden becomes overwhelming. (In particular, computation of the 2nd moments of the uncertainties requires running the model equations N times—once for each covariance column.) The most popular approach to generating uncertainties thus far has been based upon the Monte Carlo methods of generating an ensemble of disturbed solutions by perturbing initial and boundary conditions. Central difficulties lie with the choice of probability densities from which the ensemble members are generated (they are not known), and that unless the ensemble size exceeds the state vector dimension, the covariances will be singular ones.

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