Ocean Inverse Problem

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Outline:

1. Review

2. Level of no (known) motion and box inversion

3. Mapping/objective analysis

4. Simple Least Squares

5. Filtering

6. Smoothing and constraining ocean models

1 History

Modern European knowledge of the ocean began with voyages of discovery by Bartholomew Dias (1487-1488), Christopher Columbus (1492-1494), Vasco da Gama (1497-1499), Ferdinand Magellan (1519-1522), and many others. They laid the foundation for global trade routes stretching from Spain to the Philippines in the early 16th century. The routes were based on a good working knowledge of trade-winds, the westerlies, and western boundary currents in the Atlantic and Pacific (Couper, 1983: 192-193).

The early European explorers were soon followed by scientific voyages of discovery led by (among many others) James Cook (1728-1779) on the Endeavour, Resolution, and Adventure, Charles Darwin (1809-1882) on the Beagle, Sir James Clark Ross and Sir John Ross who surveyed the Arctic and Antarctic regions from the Victory, the Isabella, and the Erebus, and Edward Forbes (1815-1854) who studied the vertical distribution of life in the oceans. Others collected oceanic observations and produced useful charts, including Edmond Halley who charted the trade-winds and monsoons and Benjamin Franklin who charted the Gulf Stream.

The ocean is not well known. What we know is based on data collected from only a little more than a century of oceanographic expeditions supplemented with satellite data collected since 1978.

Slow ships of the 19th and 20th centuries gave way to satellites toward the end of the 20th century. Satellites now observe the oceans, air, and land. Their data, when fed into numerical models allows the study of Earth as a system. For the first time, we can study how biological, chemical, and physical systems interact to influence our environment.

Eras of Oceanographic Exploitation:

1. Surface Oceanography in earliest times to 1873: characterized by systematic collection of mariners observations from the deck of sailing ships. (Examples: Halley's charts of the trade-winds; Franklin s map of the Gulf Stream).

2. Deep-Sea Exploration (1873-1914) characterized by wide ranging oceanographic expeditions to survey surface and subsurface conditions near colonial claims (E.g., Challenger Expedition, Fram Expeditions).

3. International Cooperation (1957-1978) characterized by multi-national surveys of oceans and studies of oceanic processes. Examples: NORPAC cruises, the IGY cruises. Multi-ship studies of oceanic processes include MODE, POLYMODE, NORPAX, and JASIN experiments.

4. Global Observations: WOCE and satellite data: Oceanographers rely more and more on large data sets produced by others. The sets have errors and limitations which you must understand before using them.

5. Operational Oceanography.

2   Inverse Methods

Three elements of oceanography:

- Ocean observations

- Numerical models

- Theory

Those elements need to be combined for quantitative studies of the ocean and its changes. For that purpose we have to pay close attention for the differences between theory, models and observations.

Observations are essential for understanding the ocean. The basic description of the ocean is sufficient for describing the time-averaged mean circulation of the ocean, and recent work is beginning to describe the variability.

Few processes have been predicted from theory before they were observed.

A forward problem: solve a PDE given initial and boudnary conditions. Analytic or numerical solutions of dynamical equations are necessary.

An inverse problem: infer the ocean circulation, understanding it dynamically, and forecasting it, through a quantitative combination of theory and observations. Inverse methods are required to reach this goal.

To solve an inverse problem: an attempt to quantitatively test data against known dynamical principles. Need quantitative estimates and their uncertainties. In some sense the estimates of uncertainties are more important the the estimates them self.

Example:

Laplace-Poisson eq with Dirichlet boundary condition:

$$\nabla^2 \Phi = \rho \tag{1}$$

Solve for Ψ, given ρ in domain D, subject to bc $\Psi = \Psi_0$ on the boundaries δD is typical forward problem.

Well posed problem:

1. The solution exists.

2. It is unique.

3. It depends smoothly on bc's.

In general: An elliptic PDE is well posed – solution or its normal derivation are given on δD. A forward problem could be thought of as a well-posed problem of mathematical physics.

The inverse problem: find ρ given Ψ in the domain D. The problem is inverse in the sense that usual known and unknowns have been interchanged. An inverse problem is one inverse to a corresponding forward problem, interchanging the roles of at least some known and unknowns.

Both problems are posed uniquely so fare. However, in the context of noisy data such a forward problem is automatically ill posed and candidate for a solution by an inverse method.

In discrete form, the Laplace-Poisson eq. reads:

$$\Phi_{i+1,j} - 2\Phi_{i,j} + \Phi_{i,j+1} - 2\Phi_{i,j} + \Phi_{i,j-1} = \rho_{i,j} \qquad (2)$$

Assume there are $(N-2) \times (N-2)$ interior points, i.e., $(N-2) \times (N-2)$ eq. in N^2 unknowns. Adding bc $\Phi_{i,j} = \Phi_{i,j}^0$ leads to N^2 eq. in N^2 unknowns.

Note: Neumann bc: $\partial\Psi/\partial\mathbf{n}$ on boundary. With Neumann bc forward problem is under-determined: the mean is not specified. However, the inverse problem remains unchanged and well behaved.

But inverse problems are usually all under-determined in oceanography. An inverse method is suited to solve such an under-determined problem!

All illposedness owing to the lack of sufficient information is prominent in oceanography. But there are other forms of ill-posedness and are very important: too much information!

As will follow later: most or all under-determined and overdetermined problems in the presence of noisy observations can be written as:

$$\mathbf{Ex} + \mathbf{n} = \mathbf{y} \tag{3}$$

The problem is to understand the solution $\mathbf{x}$.

But $\mathbf{n}$ is a set of unknowns, too! Therefore there are always fewer eq. than unknowns. Useful inverse methods always recognize and deal with problems of imperfect data. And again: the importance of making uncertainty estimates in this context can hardly be over-estimated.

There are many reasons for using "inverse methods" in oceanography and meteorology.

- produce gridded fields (objective analysis)

- study unobserved quantities

- obtain dynamically consistent initial conditions for models.

- identify model errors.

- study observing system.

Dynamics guide here substantially the "interpolation" and allows influences of unobserved by dynamically related fields.

On the other hand: we which to use "accurate" data to correct model errors owing to inaccurate forcing fields, boundary values, initial values and dynamical parameters.

All those problems are investigated and solved using "inverse methods" (or data assimilation). There is a subtle interplay between dynamical and statistical computations, however, and we want to study both.

Meteorology refers to assimilation as the combination of a model prediction/analysis with observations with the goal to make the forecast good. Uncertainties would not be required: next day weather tells truth.

In oceanography: much attention to sensitivity of and uncertainty of the solution: we have nothing top test the solution against, since we are trying to include all information.

Literature:

Menke (1989) Gives brief elementatry account.

Taraltola (1987) Focusses on Bayesian inferences.

A. Bennett (1992) Ocean state estimation from a mathematical standpoint.

C. Wunsch (1996) Ocean state estimation problem from an observational standpoint.

I. Fukumori (2001) Data assimilation applications in oceanography.

R. Daley (1991) Atmospheric data assimilation.

3   Errors

Today oceanographers rely on large data sets produced by others. Data sets include:

- From satellites: altimetry, SST wind stress, gravimetry, SSS, ice, ...

- in situ hydrography: hydrography, XBT, P-ALACE profiles.

- Flow measurements: current meter data, float data, surface drifter.

- Tracer, nutrients, oxygen, etc.

- Surface fluxes of heat and freshwater.

Many applications use climatological (gridded) hydrographic data. All are quality controlled. Surface flux data come from ship observations, NWC.

All of those sources have errors which often are only purely known. Especially surface forcing fields have serious problems. Errors include:

- Instrument errors:

- Sampling errors:

Our knowledge about error correlations is rudimentary, and much of the future improvements of OSE will come from better understanding of data and model errors.

As compared to data, our understanding of model errors is worse. Generally it is useful to make the distinction between:

- Representation error: includes inertial oscillations, eddies, internal wave motion, etc.

- Parameterization error: includes missing or wrong physics in the model.

4   Box Inversion

The classical problem of oceanography can be described as the question of how to compute the geostrophic flow field of the ocean from observations easily made from ships. Historically one used the thermal wind relation and the major issue always was reduced to the missing integral constant.

$$\mathbf{f} \times \rho\mathbf{v} = -\nabla p \tag{4}$$

Despite the best effort of a large number of people, no adequate general method was found for the determination of the reference velocity on the space and time scale of a section obtained from a ship.

An umber of ad hoc assumptions were made:

1. geostrophic and hydrostatic balance.

2. the deep ocean is at rest.

3. the ocean is static and laminar.

4. conservation of water masses and tracers.

Lets write down the equations with convention of velocities positive north and eastward.

a) Consider the total volume moving geostrophically in to and out of an enclosed volume:

$$\sum_j^N \sum_q^Q \rho_j(q)(v_{Rj}(q) + b_j)\delta_j \Delta a_j(q) \approx 0 \qquad (5)$$

- $v_{Rj}(q)$ thermal wind in station pair j at depth interval q.

- b_j reference level velocity.

- $\Delta a_j(q)$ differential area.

- δ_j unit volume.

- (no Ekman flow).

Everything in the equation is known except b_j and a slight imbalance is anticipated due to errors.

The eq. is a discrete form of a continuous areal integral over the boundary section. It is one eq. in N unknowns b_j.

To solve it, further constraints are useful, e.g., salt conservation:

$$\sum_j^N \sum_q^Q \rho_j(q) S_j(q)(v_{Rj}(q) + b_j)\delta_j \Delta a_j(q) \approx 0 \tag{6}$$

or conservation of mass between density intervals $\rho_i < \rho < \rho_{i+1}$:

$$\sum_j^N \sum_{qi(j)}^{qi+1(j)} \rho_j(q)(v_{Rj}(q) + b_j)\delta_j \Delta a_j(q) \approx 0 \tag{7}$$

The collection of these and other similar eqt. can be written as

$$\mathbf{Ex} + \mathbf{n} = \mathbf{y} \tag{8}$$

where

$$\mathbf{x} = (b_1, b_2, ..., b_N)^T \qquad \text{reference velocity vector.} \tag{9}$$

$$\mathbf{n} = (n_1, n_2, ..., n_N)^T \qquad \text{noise vector.} \tag{10}$$

$$\mathbf{y} = (y_1, y_2, ..., y_N)^T \qquad \text{observations.} \tag{11}$$

$\mathbf{E}$ coefficient matric.

The heart of geostrophic inverse problems is the extraction of useful information from such an eq. given the fact that they are usefully under-determined (ill-conditioned inverse problems).

Inverse problems are solved in oceanography for:

1. parameter estimation: x, R

2. hypothesis testing: $y = Ex$

3. which data determine x (observing system design).

In the early days of oceanography the mathematical machinery required to deal with theses problems did not exist. Further more the presence of ocean variability on small scales makes the problem by fare more complicated. This did lead to use full ocean GCMs today.

5   Interpolation

Maps are fundamental for the interpretation of satellite data. Creating them requires always some kind of gridding and interpolation. Underlying this process is the notion that there is some of continuous function, $T(x, t)$, which we desire to reconstruct from discrete and often un-evenly sampled (gappy) and noisy data.

We need some elementary notation.

Let

$$\mathbf{R} = <y_i y_j> = \mathbf{R}(\mathbf{r}_i, \mathbf{r}_j) \tag{12}$$

be the covariance of y. If

$$R_{ij} = R(|\mathbf{r_i} - \mathbf{r}_j|) \tag{13}$$

then y is called isotropic.

Let $\mathbf{r}_0$ be a location where an interpolated value $y(\mathbf{r}_0)$ of a measurement is required:

$$\mathbf{d} = y_i + n_i \tag{14}$$

For the measurement and noise n_i holds:

$$< n(\mathbf{r}_i)n(\mathbf{r}_j) >= N(|\mathbf{r_i} - \mathbf{r}_j|) \tag{15}$$

The field we seek to map has the statistics given by $\mathbf{R}$ and the noise is uncorrelated with the value of y:

$$< y(\mathbf{r_i})\mathbf{n}(\mathbf{r}_j) >= 0 \quad all i, j \tag{16}$$

Under usual conditions the interpolated value is a weighted average of the observation

$$y(\mathbf{r_0}) = \sum_i B_j(\mathbf{r_0})d(\mathbf{r}_j) = \mathbf{B}(\mathbf{r_0})\mathbf{d} \tag{17}$$

The variance of the difference between the true value at r_0 and our interpolated value is then given by

$$E =< (y(\mathbf{r_0}) - y(\mathbf{r_0}))^2 >=< (\mathbf{B}\mathbf{d} - y(\mathbf{r_0}))^2 > \tag{18}$$

The Gauss-Markov theorem states that the minimum of the error variance is reached when $\mathbf{B}$ is chosen as

$$\mathbf{B} = \mathbf{R}(\mathbf{r}_0, \mathbf{r}_j)[\mathbf{R}(\mathbf{r}_j, \mathbf{r}_k) + N(\mathbf{r}_j, \mathbf{r}_k)]^{-1} \tag{19}$$

$$\mathbf{R}(\mathbf{r}_0, \mathbf{r}_j) = \mathbf{R}(\mathbf{r}_0, \mathbf{r}_1), \mathbf{R}(\mathbf{r}_0, \mathbf{r}_2), ..., \mathbf{R}(\mathbf{r}_0, \mathbf{r}_n) \tag{20}$$

The minimum of E is then given as

$$E_{min} = \mathbf{R}(\mathbf{r}_0, \mathbf{r}_0) - \mathbf{R}(\mathbf{r}_0, \mathbf{r}_j)[\mathbf{R}(\mathbf{r}_j, \mathbf{r}_k) + N(\mathbf{r}_j, \mathbf{r}_k)]^{-1}\mathbf{R}^T(\mathbf{r}_j, \mathbf{r}_k) \tag{21}$$

There are several important properties of the Gauss-Markov theorem.

1. No other choice of B leads to smaller errors; i.e., E is optimal.

2. No other linear combination could lead to a better estimate under the stated conditions.

A map (satellite data or anything else) is then simply a two-dimensional interpolation to a grid, sufficiently regular to be contourable, of a field that initially was observed along a swath or a track or any irregular manner. To be useful, any of this map needs to be accompanied by an estimation error map. We note that the error map depends only on the prior statistics and the data distribution, but not on the actual numbers. It can therefore be evaluated prior to any data being taken.

6   Least Squares

Let t be an independent variable which might be time or space coordinates, or simply an index. Suppose a set of measurements, e.g. $\mathbf{T}(t)$, have been made at times $t_i, i = 1, .., n$.

Suppose we have reasons to believe that there is a linear relation between T and t:

$$\mathbf{T}(t) = a + b\mathbf{t} \tag{22}$$

$$\mathbf{y}(t) = \mathbf{T}(t) + \mathbf{n}(t) = a + b\mathbf{t} + \mathbf{n}(t) \tag{23}$$

where $\mathbf{n}(t)$ is the noise and we want to determine the coefficients a and b in a least-squares manner.

The observations lead to n equations which can be written in matric notation as

$$\mathbf{Aq} = \mathbf{y} - \mathbf{n} \tag{24}$$

We are seeking a value of $\mathbf{q} = (a, b)$ that minimizes the sum-squares of the differences between $\mathbf{Aq}$ and $\mathbf{y}$:

$$min : \delta = (\mathbf{Aq} - \mathbf{y})^T(\mathbf{Aq} - \mathbf{y}) \tag{25}$$

Differentiation with respect to a and b and demanding that the derivatives vanish will

lead to

$$\mathbf{A}^{\mathbf{T}}\mathbf{A}\mathbf{q} = \mathbf{A}^{\mathbf{T}}\mathbf{y} \tag{26}$$

and

$$\mathbf{q} = (\mathbf{A}^{\mathbf{T}}\mathbf{A})^{-1}\mathbf{A}^{\mathbf{T}}\mathbf{y} \tag{27}$$

Several examples of the results are shown in the next figures and one needs to ask a great deal of questions about its meaning.

7 Filters

The early inversion application in the ocean were focused on static ocean circulation problems. However, the ocean is highly variable as satellite data show. So over the years the focus shifted from static to fully time dependent problems and from simple models to full 4-dimensional models of the ocean circulation. The extension to include one more independent coordinate - time - does not pose any principle extra problems. Rather it is just an extension of the previous methods.

The goal is to make estimates by combining a model and data - much like the previous simple least squares but now using a variety of observations and a full GCM. This is the case for many years in meteorology for weather prediction problems. In the ocean the same methods were adopted. However, the emphasis is more on hindcast and descriptions of the time-varying dynamics. This requires different approaches and foci.

If done properly, inferences from model/data combinations should be as good as any one individually or actually better than any one individually. Such model/data problems are one of statistical inferences with some powerful techniques available. However, several important stages are involved.

Stage 1 of any estimation problem has to be to understand if a physical model and the data are statistically consistent. If they are not one should stop.

A model may have adjustable parameters which can bring the model and the data into consistency and then the estimation procedure becomes an attempt to find those parameters in addition to the state. Alternatively or in addition the data error covariance matrix $\mathbf{R}(t)$ me be considered incompletely known and one can use the procedure to improve it as part of the estimation procedure (adaptive filtering).

An estimation procedure can be thought of as an interpolation in space and time: given a set of observations in space and time, use the model dynamics to estimate various state vector elements at various times of interest. Standard equations for the model and data are:

$$x(t+1) - A(t)x(t) + Bq(t) + \Gamma u(t), 0 < t < t_{f-1} \tag{28}$$

$$E(t)x(t) + n(t) = y(t), t < t < t_f \tag{29}$$

$$n(t) - 0, < n(t)n(t)^T >= R(t), < n(t)n(t') >= 0, t = t' \tag{30}$$

$$< u >= 0, < u(t)u(t)^T >= Q(t) \tag{31}$$

$$x(o) = x_0, < (x(o) - x(0))(x(o) - x(0))^T >= P(0) \tag{32}$$

This general form permits one to grapple with reality.

In the spirit of ordinary least-squares and minimum-error variance estimation, consider the general problem of finding state vectors and controls $u(t)$ that minimizes an objective function

$$
\begin{aligned}
J \;=\; & (x(0) - x_0)^T P(0)^{-1} (x(0) - x_0) + \\
& \sum (E(t)x(t) - y(t))^T R(t)^{-1} (E(t)x(t) - y(t)) \\
& + \sum u(t)^T Q(t)^{-1} u(t).
\end{aligned}
\tag{33}
$$

subject to the model constraint. I.e., we seek the state vector x and a set of controls $u(t)$, that satisfy the model and that agree with the observations with in their uncertainties provided as R and Q, respectively.

We begin with a special case: suppose we have an unbiased estimate, $x(0)$ of the state and its uncertainties, $P(0)$. How would the information available from data at time 0 be best used to make the prediction optimal for time 1? Such a computation is called Kalman filter.

There are four steps involved:

1. Make forecast using the model with the known control terms Γu set to zero.

2. Calculate the uncertainty of this forecast.

3. Do the weighted average of the forecast with the observations, the weighting being chosen to reflect the relative uncertainties.

4. Compute the uncertainties of the final weighted average.

$$\tilde{x}(t, -) = A(t-1)\tilde{x}(t-1) + B(t-1)q(t-1) \tag{34}$$

$$P(t, -) = A(t-1)P(t-1)A(t-1) + \Gamma Q(t-1)\Gamma^T \tag{35}$$

$$x(t) = \tilde{x}(r, -) + K(t)[y(t) - E(t)\tilde{x}(t, -)] \tag{36}$$

$$K(t)P(t, -)E(t)^T[E(t)P(t, -)E(t)^T + R(t)]^{-1} \tag{37}$$

$$P(t) = P(t, -) - K(t)E((t)P(t, -), t < t < t_f \tag{38}$$

The problem was reduced to finding the minimum of the cost function:

$$
\begin{aligned}
J \;=\; & (x(1,-) - x(1))^T P(1,-)^{-1}(x(1,-) - x(1)) + \\
& \sum (E(1)x(1) - y(1))^T R(1)^{-1}(E(1)x(1) - y(1))
\end{aligned}
\tag{39}
$$

8 Smoothers

Minimizing J subject to the model is still the goal. However, the strategy here is to combine all available data with the model in a "whole domain approach" to get better estimates by using data from the past and the future at the same time.

As before

$$x(t+1) - A(t)x(t) + Bq(t) + \Gamma u(t), 0 < t < t_{f-1} \tag{40}$$

$$E(t)x(t) + n(t) = y(t), t < t < t_f \tag{41}$$

$$n(t) - 0, < n(t)n(t)^T >= R(t), < n(t)n(t') >= 0, t = t' \tag{42}$$

$$< u >= 0, < u(t)u(t)^T >= Q(t) \tag{43}$$

$$x(o) = x_0, < (x(o) - x(0))(x(o) - x(0))^T >= P(0) \tag{44}$$

where Q and R are the model and data error covariances.

Similar to ordinary least squares we seek again the minimum error variance estimate (and for Gauss system maximum likelyhood estimate):

$$J = (x(0) - x_0)^T P(0)^{-1}(x(0) - x_0) + \qquad (45)$$
$$\sum (E(t)x(t) - y(t))^T R(t)^{-1}(E(t)x(t) - y(t))$$
$$+ \sum u(t)^T Q(t)^{-1} u(t).$$

subject to the model constraint.

We seek $x(t), 0 \leq T \leq t_f$, $u(t), 0 \leq T \leq t_{f-1}$ that satisfy the model and the data within their uncertainties.

As for simple LS problems we have to go back after the fact and test results and their consistency.

$$J = (x(0) - x_0)^T P(0)^{-1}(x(0) - x_0) + \qquad (46)$$
$$\sum (E(t)x(t) - y(t))^T R(t)^{-1}(E(t)x(t) - y(t))$$
$$+ \sum u(t)^T Q(t)^{-1} u(t)$$
$$-2 \sum \mu(t+1)^T [x(t+1) - Ax(t) - Bq(t) - \Gamma u(t)].$$

We turn constrained problem into unconstrained one by solving th enormal equations.

$$1/2\partial J/\partial u(t) = Q^{-1}u(t-1) + \Gamma^T\mu(t) = 0 \tag{47}$$

$$1/2\partial J/\partial\mu(t) = x(t) - Ax(t-1) - Bq(t-1) - \Gamma u(t-1) = 0 \tag{48}$$

$$1/2\partial J/\partial x(0) = P(0)^{-1}(x(0) - \tilde{x}(0)) + A^T\mu(1) = 0 \tag{49}$$

$$1/2\partial J/\partial x(t) = E(t)R(t)^{-1}[E(t)x(t) - y(t)] - \mu(t) + A^T\mu(t+1) \tag{50}$$

$$1/2\partial J/\partial x(t_f) = E(t_f)^T R(t_f)^{-1}[E(t_f)x(t_f) - y(t_f)] - \mu(t_f) = 0 \tag{51}$$

For a non-linear GCM these equations will be solved iteratively.