1

FINITE-DIMENSIONAL INVERSE THEORY

1.1 Introduction

This is an outline of some applications of finite-dimensional inverse theory to ocean modeling. The objective is not to offer a comprehensive discussion of every application and its consequences; rather it is to introduce several concepts in a relatively simple setting:

- an incomplete ocean model, based on physical laws but possessing multiple solutions;
- measurements of quantities not included in the original model but related through additional physical laws;
- inequality constraints on the model fields or the data;
- prior estimates of errors in the physical laws and the data; and
- analysis of the level of information in the system of physical laws, measurements and inequalities.

Much of this material is well covered in mathematical texts, geophysical monographs and scientific review articles. Thus the presentation is brief and directed towards subsequent application of these concepts in more complex settings. However actual oceanographic studies are discussed, and tutorial problems are posed.

1.2 The β-spiral

A major objective of physical oceanography in the 1970's was the exploration of the dynamics of mesoscale eddies and their influence on large-scale ocean circulation (Robinson, 1983). It was therefore something of a surprise when, in 1977, Stommel & Schott showed that the vertical structure of large-scale horizontal velocity fields could be explained using simple equations expressing geostrophy and mass balance. A compelling aspect of their study was the use of data in order to complete and then test their calculations. The original paper (Stommel & Schott, 1977) is somewhat cryptic. A more measured presentation may be found in the review by Olbers, Wenzel & Willebrand (1985); the latter approach will be followed here.

Consider, then, the following system of equations:

$$-\overline{\rho} f v = -p_x \,, \tag{1.2.1}$$

$$\overline{\rho} f u = -p_y \,, \tag{1.2.2}$$

$$0 = -p_z - \rho g \,, \tag{1.2.3}$$

$$\nabla \cdot \mathbf{u} + w_z = 0 \,. \tag{1.2.4}$$

These are familiar to oceanographers (Pedlosky, 1987, Chapters 2 and 3). The first two express β-plane geostrophy of a Boussinesq liquid, the third expresses the hydrostatic balance for dynamical perturbations in pressure and density while the fourth expresses conservation of volume, or mass, for a Boussinesq liquid. The common notation is: f for the Coriolis parameter; u, v and w for eastward, northward and upward velocities; x, y and z for eastward, northward and upward Cartesian coordinates; $\overline{\rho} = \overline{\rho}(z)$ and $\rho = \rho(x, y, z)$ for mean and perturbation densities, p for perturbation pressure, g for the gravitational acceleration and subscripts for partial derivatives. Vector notation will be reserved for horizontal fields and operators: $\mathbf{x} = (x, y)$, $\mathbf{u} = (u, v)$, $\nabla = \left(\frac{\partial}{\partial x}, \frac{\partial}{\partial y}\right)$. These notations will be used throughout this book.

Some well-known relations may be derived from this system. First, there are the vertically integrated thermal wind relations

$$u(\mathbf{x}, z) = u_0(\mathbf{x}) + \left(\frac{g}{f\overline{\rho}}\right) \int_{z_0}^{z} \rho_y(\mathbf{x}, \zeta) d\zeta \,, \tag{1.2.5}$$

$$v(\mathbf{x}, z) = v_0(\mathbf{x}) - \left(\frac{g}{f\overline{\rho}}\right) \int_{z_0}^{z} \rho_x(\mathbf{x}, \zeta) d\zeta \,, \tag{1.2.6}$$

or simply

$$\mathbf{u}(\mathbf{x}, z) = \mathbf{u}_0(\mathbf{x}) + \mathbf{u}'(\mathbf{x}, z) \,, \tag{1.2.7}$$

where $\mathbf{u}_0$ is the horizontal velocity at depth z_0, while $\mathbf{u}'$ is determined by the density field. Second, there is the Sverdrup interior vorticity balance:

$$w_z = \frac{\beta v}{f}\,, \tag{1.2.8}$$

where β is the northward gradient of the Coriolis parameter: $f = f(y) = f_* + \beta(y - y_*)$ for y close to some local latitude y_*. These relations would not determine the velocity field $(\mathbf{u}, w)$, even if the density field ρ were known. However, the indeterminacy is only that of unknown fields at a single depth, namely $\mathbf{u}(\mathbf{x}, z_0)$ and $w(\mathbf{x}, z_0)$. Stommel & Schott showed that these unknown reference fields may be estimated by assuming the availability of measurements of some conservative tracer ϕ, satisfying the steady-state conservation law

$$\mathbf{u} \cdot \boldsymbol{\nabla}\phi + w\phi_z = 0\,. \tag{1.2.9}$$

The tracer ϕ might be salinity S or potential temperature θ (Pedlosky, 1987, Chapter 1) or some function of them both: $F = F(S, \theta)$, such as potential density. Combining the vertical derivative of (1.2.9) with (1.2.7) and (1.2.8) yields

$$(\mathbf{u} \cdot \boldsymbol{\nabla} + w\frac{\partial}{\partial z})(f\phi_z) = (g/\overline{\rho})\,J\,, \tag{1.2.10}$$

where $J(\rho, \phi) = \rho_x\phi_y - \rho_y\phi_x$. The quantity $f\phi_z$ is a potential vorticity which would be conserved if ρ were itself conserved: see Eliassen & Kleinschmidt (1957) for a comprehensive discussion. The tracer equation (1.2.9) may be used again to eliminate the vertical velocity w:

$$\mathbf{u} \cdot \mathbf{a} = (g/\overline{\rho})\,J(\rho, \phi)\,, \tag{1.2.11}$$

where the vector $\mathbf{a}$ is given by

$$\mathbf{a}(\mathbf{x}, z) = \boldsymbol{\nabla}(f\phi_z) - \frac{\boldsymbol{\nabla}\phi}{\phi_z}\, f\phi_{zz}\,. \tag{1.2.12}$$

Finally, using the integrated thermal wind relations (1.2.7) yields

$$\mathbf{u}_0 \cdot \mathbf{a} = c\,, \tag{1.2.13}$$

where

$$c(\mathbf{x}, z) = -\mathbf{u}' \cdot \mathbf{a} + (g/\overline{\rho})\, J(\rho, \phi)\,. \tag{1.2.14}$$

Now $\mathbf{a}$ and c depend upon g, $\overline{\rho}$, f, $\boldsymbol{\nabla}\rho$, $\boldsymbol{\nabla}\phi$, ϕ_z and ϕ_{zz} and so are measurable, in principle, using closely spaced hydrographic stations (e.g., Pickard & Emery, 1990). Consequently, the horizontal reference velocity $\mathbf{u}_0$ may be measured indirectly, using the hydrographic data. Since (1.2.13) holds at all levels, any two levels may be chosen to determine the two components u_0 and v_0. Then the vertical velocity w may be determined using the tracer equation (1.2.9). All that would remain would be the choice of a pair of levels, and provided the model physics are realistic, the solution for $\mathbf{u}_0$ should be independent of the choice. However, (1.2.13) is not an exact relation, being derived from the approximate dynamical laws (1.2.1)–(1.2.4), (1.2.9), and the data will contain experimental errors. Consequently the estimate of $\mathbf{u}_0$ from (1.2.13) should be a best fit using data from at least two levels.

Suppose N levels are chosen ($N \geq 2$). Let $c_n = c(\mathbf{x}, z_n)$ and $\mathbf{a}_n = \mathbf{a}(\mathbf{x}, z_n)$ for $1 \leq n \leq N$. Then a simple least-squares best fit minimizes

$$R^2 \equiv \sum_{n=1}^{N} R_n^2 \equiv \sum_{n=1}^{N} (c_n - \mathbf{u}_0 \cdot \mathbf{a}_n)^2\,, \tag{1.2.15}$$

where R_n is the residual at the nth level and R is the root-mean-square (rms) total error. It is a trivial exercise to show that R^2 is least if $\mathbf{u}_0$ satisfies a simple linear system:

$$\mathbf{M}\mathbf{u}_0 = \mathbf{d}\,, \tag{1.2.16}$$

where the 2×2 symmetric, non-negative matrix $\mathbf{M}$ depends upon the components of $\mathbf{a}_n$, while $\mathbf{d}$ depends upon $\mathbf{a}_n$ and c. So (1.2.16) would seem to yield an estimate of the reference velocity $\mathbf{u}_0$. However, adding levels works only if the coefficient vector $\mathbf{a}$ appearing in the left-hand side of (1.2.13) is significantly depth-dependent. Otherwise there is effectively only one indirect observation of the vector $\mathbf{u}_0$ at each station $\mathbf{x}$. If $\mathbf{a}$ or c varies with depth, then (1.2.11) immediately implies that the total velocity vector $\mathbf{u}$ also depends on depth, that is, the large-scale ocean current performs a vertical spiral at each station.

Before proceeding to examine Stommel & Schott's results, it is necessary to explain their terse formulation. Assuming that ρ itself suffices as a near-conservative tracer and, neglecting $(\rho\rho_{zz}/\rho_z^2)$, reduces (1.2.10) to

$$uf\rho_{zx} + v(f\rho_{zy} + \beta\rho_z) \cong 0\,. \tag{1.2.17}$$

Let $z = h(\mathbf{x}, \rho)$ denote a surface of constant density. On this surface,

$$\boldsymbol{\nabla}\rho + \rho_z \boldsymbol{\nabla} h = 0\,. \tag{1.2.18}$$

Once more neglecting second vertical derivatives of ρ, and combining (1.2.17), (1.2.18) leads to

$$uh_{xz} + v\left(h_y - \frac{\beta z}{f}\right)_z = 0\,, \tag{1.2.19}$$

which is Stommel & Schott's equation (1). The field h_{xz}, for example, may be evaluated as $\rho_z\, h_{x\rho}$. Again, this holds for the depth h of each isopycnal surface, and holds at each station $\mathbf{x}$.

Hydrographic data from *Atlantis* Stations 5754–5764 at 28°N, *Discovery* Stations 3594–3607 at 24°N and *Discovery* Stations 3627–3641 at 32°N were used by Stommel & Schott to estimate $\mathbf{u}_0$ for a reference level at $z_0 = 1000$ m depth. They obtained $u_0 = 0.0034 \pm .0003$ m s^{-1}, $v_0 = 0.006 \pm .00013$ m s^{-1} at 28°N, 36°W, the errors being the standard errors for the linear fit.

The spiral for the horizontal velocity $\mathbf{u}$ at 28°N, 36°W is shown in Fig. 1.2.1. A profile for the vertical velocity w was also obtained; a negative value for w was found at the surface, consistent with the local value of the wind stress curl (Pedlosky, 1987, Chapter 4). Stommel & Schott then "tested" their circulation model by calculating the minimal value of the squared residual R^2 for incorrect values of the Coriolis parameter f appearing in (1.2.19). They normalized R with respect to the inhomogeneous term in their equation for $\mathbf{u}_0$, that is, with respect to the analogue of c in (1.2.13): see Fig. 1.2.2. The residual finds a clear minimum for the correct value of f at 28°N, indicating that the "the density field in the ocean senses its latitude."

The β-spiral theory includes two of the concepts essential to inverse methods. First, there is the incomplete set of physical laws (1.2.1)–(1.2.4) or their rearrangement as (1.2.7) and (1.2.8), exposing the indeterminate reference velocity. Second, there is the indirect measurement of an additional quantity, in this case a conserved tracer.

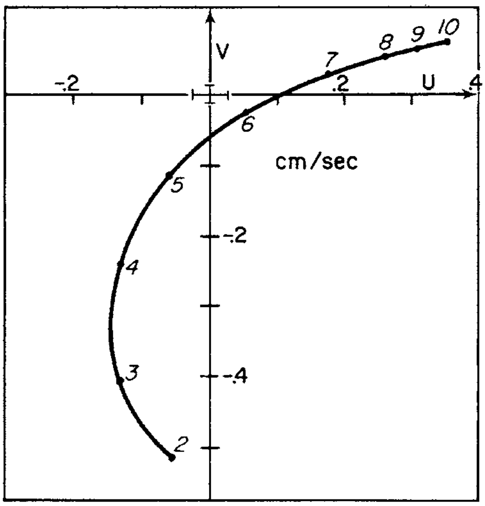

Figure 1.2.1. The β-spiral in horizontal velocity $\mathbf{u} = \mathbf{u}(z)$ at 28°N, 36°W. Depths in 100 meters; error bars at the origin (after Stommel & Schott, 1977).

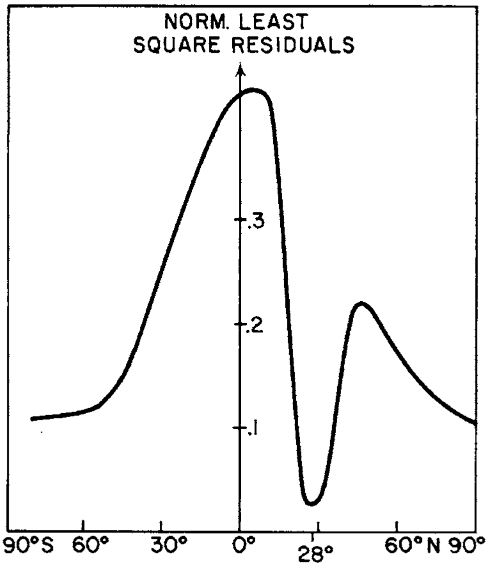

Figure 1.2.2. Normalized least-squares residual for 28°N, 36°W. Density data computed for various values of latitude (after Stommel & Schott, 1977). Note that the minimal square value is about 0.02, so the minimal rms value is about 0.14.

What are most conspicuously absent are prior estimates of the errors in the final dynamical equation (1.2.13), and of the errors in the hydrographic data. Were the variances of these errors known to vary with depth, it would be appropriate to seek a non-uniformly weighted least-squares fit, instead of the uniformly weighted fit (1.2.15). Moreover, comparison of the residual with prior estimates would, in effect, test the several hypotheses tacitly included in the β-spiral theory. For example, the minimal normalized rms residual at 28°N is, judging from Fig. 1.2.2, about 0.14. Such a value is somewhat larger than the order of the Rossby number or scale estimate for the mesoscale variability neglected in (1.2.1)–(1.2.2). The value is comparable with estimates of relative data error. Stommel & Schott concluded their study by remarking that the simple dynamics could be augmented by including diffusion in the tracer conservation law, the eddy diffusivity being chosen by the least-squares approach. The suggestion has been explored at length, and the reader is referred to Olbers *et al.* (1985) for a very detailed analysis of the North Atlantic circulation along these lines. A careful discussion of β-spiral concepts may be found in Stommel (1987).

Exercise 1.2.1 Make scale estimates of the errors in the approximate dynamics of the β-spiral. □

Exercise 1.2.2 Derive the forms of matrix $\mathbf{M}$ and vector $\mathbf{d}$ in (1.2.16). Verify that $\mathbf{M}$ is symmetric and non-negative. Under what conditions is $\mathbf{M}$ singular? □

1.3 Wunsch's method: a first analysis

At the same time that Stommel & Schott were estimating reference velocities locally from hydrographic data, Wunsch (1977) showed that reference velocities could be estimated simultaneously around a closed path in the ocean. His investigation was prompted by Worthington's inability to find a uniform depth of no motion in the North Atlantic consistent with geostrophy and the conservation of total heat and salt at various levels (Worthington, 1976).

Again the unknown reference velocity is $\mathbf{u}_0$ in (1.2.7), the thermal wind $\mathbf{u}'$ being known from hydrographic data. By construction, $\mathbf{u}' = \mathbf{0}$ at the reference level z_0 which in general may be chosen to depend upon position: $z_0 = z_0(\mathbf{x})$. Wunsch chose the reference level to be the ocean bottom at $z_0(\mathbf{x}) = H(\mathbf{x})$, so $\mathbf{u}_0(\mathbf{x})$ was defined to

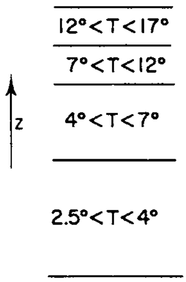

Figure 1.3.1. Subdivision of water column into layers defined by temperature ranges (after Worthington, 1976).

be the bottom velocity. Guided by Worthington's classical water mass classifications, Wunsch divided the water column everywhere into a number of layers (see Fig. 1.3.1) defined by temperature ranges. These layers need not have the same thickness at each station. The stations used by Wunsch, together with the U.S. coastline, form a closed path in the Western North Atlantic (Fig. 1.3.2). Let v now denote the outward velocity across the sections; thus $v = \mathbf{u} \cdot \mathbf{n}$ where $\mathbf{n}$ is the outward unit normal. In particular, let $v' = \mathbf{u}' \cdot \mathbf{n}$ be the outward thermal wind, and let $b = \mathbf{u}_0 \cdot \mathbf{n}$ be the outward velocity at the bottom. Let $v_n'(z)$ and b_n denote the thermal wind estimate and unknown bottom velocity midway between the nth station pair, where $1 \le n \le N$, and let $\overline{v}'_{mn}$ denote the average value of v_n' in the mth layer of the water column, where $1 \le m \le M$. Wunsch chose the Mth layer to be the total water column, thus the Mth tracer is the total mass of the column. The assumptions of tracer conservation within each layer are

$$\sum_{n=1}^{N} (\overline{v}'_{mn} + b_n)\Delta z_{mn}\Delta x_n = 0\,, \qquad (1 \le m \le M)\,, \tag{1.3.1}$$

where Δz_{mn} is the thickness of the mth layer at the nth station pair, while Δx_n is the separation of the nth station pair. This system of M equations for the N unknowns b_n, $1 \le n \le N$, may be written in matrix notation as

$$\mathbf{A}\mathbf{b} = \mathbf{c}\,, \tag{1.3.2}$$

where $\mathbf{A}$ is an $M \times N$ matrix with elements $A_{mn} = \Delta z_{mn}\Delta x_n$, while $\mathbf{c}$ is a column vector of length M with elements $c_m = -\sum_{n=1}^{N} \overline{v}'_{mn} A_{mn}$.

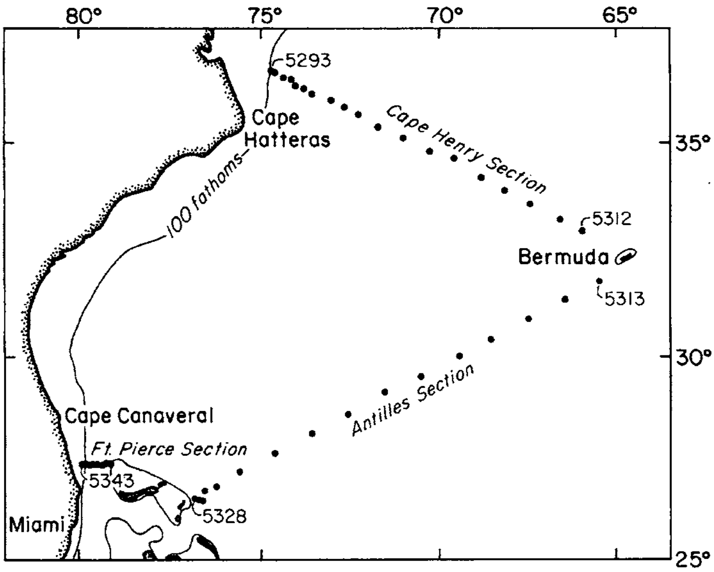

Figure 1.3.2. Locations of *Atlantis* 215 Stations used by Wunsch (after Wunsch, 1977).

Wunsch chose $M = 5$ layers defined by the four temperature ranges 12° to 17°C, 7° to 12°C, 4° to 7°C, 2.5° to 4°C, and by the total mass. The hydrographic data were comprised of $N = 43$ station pairs. Thus (1.3.2) represents 5 equations for the 43 unknown bottom velocities b_j, and would seem to be an underdetermined system having many solutions.

Somewhat arbitrarily, Wunsch chose the smallest solution, that is, the vector $\mathbf{b}$ of smallest length $(\mathbf{b}^*\mathbf{b})^{1/2}$ where superscript $*$ denotes the transpose. Minimization of the length of $\mathbf{b}$, subject to the linear constraint (1.3.2), may be achieved by minimizing the quadratic form $\mathcal{J}_1$ defined by

$$\mathcal{J}_1 = \mathbf{b}^*\mathbf{b} + 2\boldsymbol{\lambda}^*(\mathbf{A}\mathbf{b} - \mathbf{c}) = \mathcal{J}_1[\mathbf{b}, \boldsymbol{\lambda}] . \tag{1.3.3}$$

In (1.3.3) the constraint (1.3.2) has been appended to the squared length using an unknown Lagrange multiplier $\boldsymbol{\lambda}$, which is a column vector of length M. The factor of 2 is included for later convenience. It is a simple exercise to show that $\mathcal{J}_1$, as a function of $\mathbf{b}$ and $\boldsymbol{\lambda}$, is least if

$$\mathbf{b} + \mathbf{A}^*\boldsymbol{\lambda} = 0 \tag{1.3.4}$$

and, as required, (1.3.2) holds. Further simple manipulations yield the sought-after smallest solution:

$$\mathbf{b} = \mathbf{A}^*(\mathbf{A}\mathbf{A}^*)^{-1}\mathbf{c}\,, \tag{1.3.5}$$

which clearly satisfies (1.3.2). Note that the symmetric matrix $\mathbf{A}\mathbf{A}^*$ has dimension $M \times M$, and is non-negative. However, it may be singular, and so (1.3.5) is at best a formal solution. The difficulty may be overcome by admitting errors in the hydrography and conservation laws, that is, by not seeking exact satisfaction of (1.3.2). This may be accomplished by replacing (1.3.3) with the quadratic form

$$\mathcal{J}_2 = W_1\mathbf{b}^*\mathbf{b} + W_2(\mathbf{A}\mathbf{b} - \mathbf{c})^*(\mathbf{A}\mathbf{b} - \mathbf{c}) = \mathcal{J}_2[\mathbf{b}]\,, \tag{1.3.6}$$

where W_1 and W_2 are positive weights. The *strong constraint* (1.3.2), appended to the penalty function (1.3.3) using a Lagrange multiplier, has been replaced by a *weak constraint* which may be satisfied, at the expense of minimizing the length of $\mathbf{b}$, by increasing the ratio W_2/W_1. It is readily shown that (1.3.6) is minimized by

$$\mathbf{b} = (\mathbf{A}^*\mathbf{A} + (W_1/W_2)\mathbf{I})^{-1}\mathbf{A}^*\mathbf{c}\,, \tag{1.3.7}$$

or, equivalently,

$$\mathbf{b} = \mathbf{A}^*(\mathbf{A}\mathbf{A}^* + (W_1/W_2)\mathbf{I})^{-1}\mathbf{c}\,, \tag{1.3.8}$$

where $\mathbf{I}$ is the $N \times N$ unit matrix in (1.3.7), but is the $M \times M$ matrix in (1.3.8). Since the weights are positive, the matrix inverses in (1.3.7) and (1.3.8) are well defined, so a unique solution has been obtained.

It is instructive to examine (1.3.8) in its limits. If the hydrographic data and conservation laws are perfect, then $(W_2/W_1) \to \infty$, and (1.3.5) and (1.3.2) are recovered. If the data are worthless or the laws invalid, then $(W_2/W_1) \to 0$ and so $\mathbf{b} \to \mathbf{0}$. That is, no