Inverse Modeling of the Ocean and Atmosphere

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Chapter 1

Variational assimilation

Chapter 1 is a minimal course on assimilating data into models using the calculus of variations. The theory is introduced with a "toy" model in the form of a single linear partial differential equation of first order. The independent variables are a spatial coordinate, and time. The well-posedness of the mixed initial-boundary value problem or "forward model" is established, and the solution is expressed explicitly with the Green's function. The introduction of additional data renders the problem ill-posed. This difficulty is resolved by seeking a weighted least-squares best fit to all the information. The fitting criterion is a penalty functional that is quadratic in all the misfits to the various pieces of information, integrated over space and time as appropriate. The best-fit or "generalized inverse" is expressed explicitly with the representers for the penalty functional, and with the Green's function for the forward model. The behavior of the generalized inverse is examined for various limiting choices of weights. The smoothness of the inverse is seen to depend upon the nature of the weights, which will be subsequently identified as kernel inverses of error covariances. After reading Chapter 1, it is possible to carry out the first four computing exercises in Appendix A.

1.1 Forward models

1.1.1 Well-posed problems

Mechanics is captured mathematically by "well-posed problems". The mechanical laws for particles, rigid bodies and fields are with few exceptions expressed as ordinary or partial differential equations; data about the state of the mechanical system are provided in initial conditions or boundary conditions or both. The collection of general equations and ancillary conditions constitute a "well-posed problem" if, according to Hadamard (1952; Book I) or Courant and Hilbert (1962; Ch. III, §6):

(i) a solution exists,

which

(ii) is uniquely determined by the inputs (forcing, initial conditions, boundary conditions),

and which

(iii) depends continuously upon the inputs.

Classical particles and bodies move smoothly, while classical fields vary smoothly so only differentiable functions qualify as solutions. The repeatability of classical mechanics argues for determinism. The classical perception of only finite changes in a finite time argues for continuous dependence.

Ill-posed problems fail to satisfy at least one of conditions (i)–(iii). They cannot be solved satisfactorily but can be resolved by generalized inversion, which is the subject of this chapter. Inevitably, well-posed problems are also known as "forward models": given the dynamics (the mechanical laws) and the inputs (any initial values, boundary values or sources), find the state of the system. In this first chapter, an example of a forward model is given; the uniqueness of solutions is proved, and an explicit solution is constructed using the Green's function. That is, the well-posedness of the forward model is established.

1.1.2 A "toy" example

The following "toy" example involves an unknown "ocean circulation" $u = u(x, t)$, where x, t and u are real variables. The "ocean basin" is the interval $0 \le x \le L$, while the time of interest is $0 \le t \le T$: see Fig. 1.1.1.

The "ocean dynamics" are expressed as a linear, first-order partial differential equation:

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = F \tag{1.1.1}$$

for $0 \le x \le L$ and $0 \le t \le T$, where c is a known, constant, positive phase speed. The inhomogeneity $F = F(x, t)$ is a specified forcing field; later it will become known as the prior estimate of the forcing. An initial condition is

$$u(x, 0) = I(x) \tag{1.1.2}$$

for $0 \le x \le L$, where I is specified. A boundary condition is

$$u(0, t) = B(t) \tag{1.1.3}$$

for $0 \le t \le T$, where B is specified.

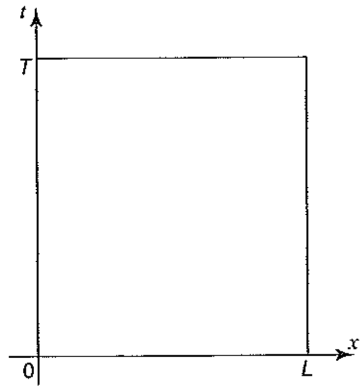

Figure 1.1.1 Toy ocean basin.

1.1.3 Uniqueness of solutions

To determine the uniqueness of solutions (Courant and Hilbert, 1962) for (1.1.1), (1.1.2) and (1.1.3), let u_1 and u_2 be two solutions for the same choices of F, I and B. Define the difference

$$v \equiv u_1 - u_2. \tag{1.1.4}$$

Then

$$\frac{\partial v}{\partial t} + c\frac{\partial v}{\partial x} = 0 \tag{1.1.5}$$

for $0 \le x \le L$ and $0 \le t \le T$;

$$v(x, 0) = 0 \tag{1.1.6}$$

for $0 \le x \le L$, and

$$v(0, t) = 0 \tag{1.1.7}$$

for $0 \le t \le T$.

Multiplying (1.1.5) by v and integrating over all x yields

$$\frac{d}{dt}\frac{1}{2}\int_0^L v^2\,dx = -c\left[\frac{1}{2}v^2\right]_{x=0}^{x=L} = -\frac{c}{2}v(L, t)^2, \tag{1.1.8}$$

using the boundary condition (1.1.7). Integrating (1.1.8) over time from 0 to t yields

$$\frac{1}{2}\int_0^L v^2(x, t)\,dx = \frac{1}{2}\int_0^L v^2(x, 0)\,dx - \frac{c}{2}\int_0^t v^2(L, s)\,ds. \tag{1.1.9}$$

The right-hand side (rhs) of (1.1.9) is nonpositive, as a consequence of the initial condition (1.1.6). Hence

$$v(x, t) = 0, \tag{1.1.10}$$

that is,

$$u_1(x,t) = u_2(x,t) \tag{1.1.11}$$

for $0 \le x \le L$ and $0 \le t \le T$. So we have established that (1.1.1), (1.1.2) and (1.1.3) have a unique solution for each choice of F, I and B.

1.1.4 Explicit solutions: Green's functions

We may construct the solution explicitly, using the Green's function (Courant and Hilbert, 1953) or fundamental solution γ for (1.1.1)–(1.1.3).

Let $\gamma = \gamma(x,t,\xi,\tau)$ satisfy

$$-\frac{\partial \gamma}{\partial t} - c\frac{\partial \gamma}{\partial x} = \delta(x-\xi)\delta(t-\tau), \tag{1.1.12}$$

where the δs are Dirac delta functions, and $0 \le \xi \le L$, $0 \le \tau \le T$. Also,

$$\gamma(L,t,\xi,\tau) = 0 \tag{1.1.13}$$

for $0 \le t \le T$, and

$$\gamma(x,T,\xi,\tau) = 0 \tag{1.1.14}$$

for $0 \le x \le L$.

Exercise 1.1.1

(a) Verify that

$$\gamma(x,t,\xi,\tau) = \delta(x - \xi - c(t-\tau))H(\tau - t) \tag{1.1.15}$$

for $0 \le x < L,\ 0 \le t \le T$, where H is the Heaviside unit step function.

(b) Show that

$$u(\xi,\tau) = u_F(\xi,\tau) \equiv \int_0^T dt \int_0^L dx\, \gamma(x,t,\xi,\tau)F(x,t) + \int_0^L dx\, \gamma(x,0,\xi,\tau)I(x) + c\int_0^T dt\, \gamma(0,t,\xi,\tau)B(t). \tag{1.1.16}$$

□

Relabeling (1.1.16) yields

$$u_F(x,t) = \int_0^T d\tau \int_0^L d\xi \gamma(\xi,\tau,x,t)F(\xi,\tau) + \int_0^L d\xi \gamma(\xi,0,x,t)I(\xi) + c\int_0^T d\tau \gamma(0,\tau,x,t)B(\tau), \tag{1.1.17}$$

which is an explicit solution for the "forward model". It is also the prior estimate or "first-guess" or "background" for u.

Note 1. By inspection, u_F depends continuously upon changes to F, I and B; if these change by $O(\epsilon)$, so does u_F.

Note 2. We actually require $I(0) = B(0)$, or else u_F is discontinuous across the phase line $x = ct$, for all t.

We conclude that the forward model (1.1.1)–(1.1.3) is well-posed. Any additional information would overdetermine the system, and a smooth solution would not exist.

Exercise 1.1.2

Code the finite-difference equation

$$u_n^{k+1} = u_n^k - c(\Delta t/\Delta x)\left(u_n^k - u_{n-1}^k\right) + \Delta t F_n^k, \tag{1.1.18}$$

where $u_n^k = u(n\Delta x, k\Delta t)$, etc. Perform some numerical integrations. Derive and verify experimentally the Courant–Friedrichs–Lewy stability criterion (Haltiner and Williams, 1980). □

Exercise 1.1.3

Slow, one-dimensional viscous flow $u = u(x, t)$ is approximately governed by

$$\frac{\partial u}{\partial t} = \nu \frac{\partial^2 u}{\partial x^2} - \rho^{-1} \frac{\partial p}{\partial x}, \tag{1.1.19}$$

where ν is the uniform kinematic viscosity, ρ is the uniform density and $p = p(x, t)$ is the externally imposed pressure gradient. Consider an infinite domain: $-\infty < x < \infty$, and a finite time interval: $0 < t < T$. A suitable initial condition is

$$u(x, 0) = I(x). \tag{1.1.20}$$

Assume that both $\partial p/\partial x$ and I vanish as $|x| \to \infty$.

(a) Derive the following energy integral when both $\partial p/\partial x$ and I vanish everywhere:

$$\frac{d}{dt}\frac{1}{2}\int_{-\infty}^{\infty} u^2\, dx = -\frac{\nu}{2}\int_{-\infty}^{\infty}\left(\frac{\partial u}{\partial x}\right)^2 dx. \tag{1.1.21}$$

Hence prove that there is at most one solution for each choice of p and I.

(b) Show that the solution of (1.1.19), (1.1.20) is

$$u(x, t) = -\rho^{-1}\int_0^T d\tau \int_{-\infty}^{\infty} d\xi\, \phi(\xi, \tau, x, t)\frac{\partial p}{\partial x}(\xi, \tau) + \int_{-\infty}^{\infty} d\xi\, \phi(\xi, 0, x, t) I(\xi), \tag{1.1.22}$$

where the Green's function or fundamental solution $\phi(x, t, \xi, \tau)$ satisfies

$$-\frac{\partial \phi}{\partial t} = \nu \frac{\partial^2 \phi}{\partial x^2} + \delta(x - \xi)\delta(t - \tau), \tag{1.1.23}$$

subject to

$$\phi(x, T, \xi, \tau) = 0 \tag{1.1.24}$$

for $-\infty < x < \infty$, and

$$\phi(x, t, \xi, \tau) \to 0 \tag{1.1.25}$$

as $|x| \to \infty$.

(c) Verify that

$$\phi(x, t, \xi, \tau) = \frac{H(\tau - t)e^{\frac{-(x-\xi)^2}{2\nu(t-\tau)}}}{\sqrt{2\pi\nu(t - \tau)}}. \tag{1.1.26}$$

Notice that the effective range of integration with respect to time in (1.1.22) is $0 < \tau < t$. □

Exercise 1.1.4

(1) Is quantum mechanics captured mathematically as well-posed problems? See, for example, Schiff (1949, p. 48).
(2) Can well-posed problems have chaotic solutions? □

1.2 Inverse models

1.2.1 Overdetermined problems

We shall spoil the well-posedness of the forward model examined in §1.1, by introducing additional information about the toy "ocean circulation" field $u(x, t)$. This information will consist of imperfect observations of u at isolated points in space and time, for the sake of simplicity. The forward model becomes overdetermined; it cannot be solved with smooth functions and must be regarded as ill-posed. We shall resolve the ill-posed problem by constructing a weighted, least-squares best-fit to all the information. It will be shown that this best-fit or "generalized inverse" of the ill-posed problem obeys the Euler–Lagrange equations.

1.2.2 Toy ocean data

Let us assume that a finite number M of measurements (observations, data, ...) of u were collected in the bounded "ocean basin" $0 \le x \le L$, during the "cruise" $0 \le t \le T$. The data were collected at the points (x_m, t_m), where $1 \le m \le M$: see Fig. 1.2.1. The

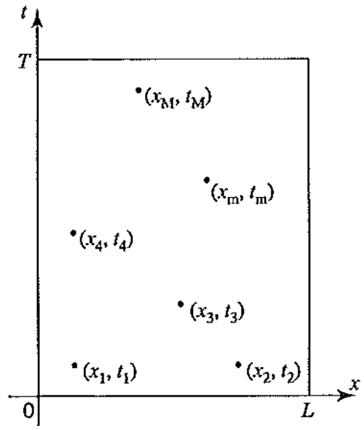

Figure 1.2.1 Toy ocean data.

data are related to the "true" ocean circulation field $u(x, t)$ by

$$d_m = u(x_m, t_m) + \epsilon_m, \tag{1.2.1}$$

$1 \leq m \leq M$, where d_m is the datum or recorded value, and $u(x_m, t_m)$ is the true value of the circulation. The measurement error ϵ_m may arise from an imperfect measuring system, or else from mistakenly identifying streamfunction and pressure, for example. On the other hand, if our ocean model were quasigeostrophic and the data included internal waves, then there would also be cause to admit errors in the dynamics.

1.2.3 Failure of the forward solution

Let us now consider how these data relate to the forward problem. If $u_F = u_F(x, t)$ is the forward solution:

$$\frac{\partial u_F}{\partial t} + c\frac{\partial u_F}{\partial x} = F \tag{1.2.2}$$

for $0 \leq x \leq L$ and $0 \leq t \leq T$, with

$$u_F(x, 0) = I(x) \tag{1.2.3}$$

for $0 \leq x \leq L$, and

$$u_F(0, t) = B(t) \tag{1.2.4}$$

for $0 \leq t \leq T$, then we may expect that

$$u_F(x_m, t_m) \neq d_m \tag{1.2.5}$$

for at least some m: $1 \leq m \leq M$. We therefore assume that there are errors in our prior estimates for F, I and B. So the true circulation u must satisfy

$$\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} = F + f \tag{1.2.6}$$

for $0 \le x \le L$ and $0 \le t \le T$,

$$u(x,0) = I(x) + i(x) \tag{1.2.7}$$

for $0 \le x \le L$ and

$$u(0,t) = B(t) + b(t) \tag{1.2.8}$$

for $0 \le t \le T$. Note that what is implied to be a forcing error $f = f(x,t)$ on the rhs of (1.2.6) may actually be an error in the dynamics expressed on the left-hand side (lhs) of (1.2.6).

1.2.4 Least-squares fitting: the penalty functional

We have established that for any choice of $F + f$, $I + i$ and $B + b$, there is a unique solution for u. However, we have only the M data values d_m to guide us and so the error fields f, i and b are undetermined, while the data errors ϵ_m are unknown. We shall seek the field $\hat{u} = \hat{u}(x,t)$ that corresponds to the smallest values for f, i, b and ϵ_m in a weighted, least-squares sense. Specifically, we shall seek the minimum of the quadratic *penalty functional* or *cost functional* $\mathcal{J}$:

$$\mathcal{J} = \mathcal{J}[u] \equiv W_f \int_0^T dt \int_0^L dx\, f(x,t)^2 + W_i \int_0^L dx\, i(x)^2 + W_b \int_0^T dt\, b(t)^2 + w \sum_{m=1}^{M} \epsilon_m^2, \tag{1.2.9}$$

where W_f, W_i, W_b and w are positive weights that we are free to choose. There are more general quadratic forms, but (1.2.9) will suffice for now. The lhs of (1.2.9) expresses the dependence of $\mathcal{J}$ upon u, while the rhs only involves f, i, b and ϵ_m. It is to be understood that the latter are the values that would be obtained, were u substituted into (1.2.1) and (1.2.6)–(1.2.8). These *definitions* could be appended to $\mathcal{J}$ using Lagrange multipliers, but it is simpler just to remember them ourselves. Finally, note that while u is a *field* of values for $0 \le x \le L$ and $0 \le t \le T$, the penalty functional $\mathcal{J}[u]$ is a *single number* for each choice of the *entire field* u.

Rewriting (1.2.9), with f, i, b and ϵ_m replaced by their definitions, yields

$$\begin{aligned}\mathcal{J}[u] = {} & W_f \int_0^T dt \int_0^L dx \left\{ \frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} - F \right\}^2 + W_i \int_0^L dx\, \{u(x,0) - I(x)\}^2 \\ & + W_b \int_0^T dt\, \{u(0,t) - B(t)\}^2 + w \sum_{m=1}^{M} \{u(x_m, t_m) - d_m\}^2 .\end{aligned} \tag{1.2.10}$$

The dependence upon u (and upon F, I, B and d_m) is now explicit.

1.2.5 The calculus of variations: the Euler–Lagrange equations

We shall use the calculus of variations (Courant and Hilbert, 1953; Lanczos, 1966) to find a *local extremum* of $\mathcal{J}$. Since $\mathcal{J}$ is quadratic in u and clearly nonnegative, the local extremum must be the global minimum. To begin, let $\hat{u} = \hat{u}(x, t)$ be the local extremum. That is,

$$\mathcal{J}[\hat{u} + \delta u] = \mathcal{J}[\hat{u}] + O(\delta u)^2 \tag{1.2.11}$$

for some small change $\delta u = \delta u(x, t)$. This statement can be made more precise but we shall proceed informally:

$$\begin{aligned}
\delta\mathcal{J} &\equiv \mathcal{J}[\hat{u} + \delta u] - \mathcal{J}[\hat{u}] \\
&= 2W_f \int_0^T dt \int_0^L dx \left\{ \frac{\partial \hat{u}}{\partial t} + c\frac{\partial \hat{u}}{\partial x} - F \right\} \left\{ \frac{\partial \delta u}{\partial t} + c\frac{\partial \delta u}{\partial x} \right\} \\
&\quad + 2W_i \int_0^L dx\ \{\hat{u}(x, 0) - I(x)\}\, \delta u(x, 0) + 2W_b \int_0^T dt\ \{\hat{u}(0, t) - B(t)\} \delta u(0, t) \\
&\quad + 2w \sum_{m=1}^{M} \{\hat{u}(x_m, t_m) - d_m\} \delta u(x_m, t_m) + O(\delta u)^2 .
\end{aligned} \tag{1.2.12}$$

Note 1. F, I, B and d_m have not been allowed to vary; only $\hat{u}$ has been varied.
Note 2. We have assumed that

$$\delta \frac{\partial u}{\partial t}(x, t) = \frac{\partial \delta u}{\partial t}(x, t), \quad \text{etc.} \tag{1.2.13}$$

The lhs of (1.2.13) is a variation of $(\partial u/\partial t)$; the rhs is the time derivative of the variation of u.

For convenience let us introduce the field $\lambda = \lambda(x, t)$:

$$\lambda \equiv W_f \left(\frac{\partial \hat{u}}{\partial t} + c\frac{\partial \hat{u}}{\partial x} - F \right). \tag{1.2.14}$$

Then the first term in $\delta\mathcal{J}$ is

$$\begin{aligned}
&2 \int_0^T dt \int_0^L dx\, \lambda \left\{ \frac{\partial \delta u}{\partial t} + c\frac{\partial \delta u}{\partial x} \right\} \\
&= 2 \left[\int_0^L dx\, \lambda \delta u \right]_{t=0}^{t=T} + 2 \left[\int_0^T dt\, \lambda c \delta u \right]_{x=0}^{x=L} \\
&\quad + 2 \int_0^T dt \int_0^L dx \left\{ -\frac{\partial \lambda}{\partial t} - c\frac{\partial \lambda}{\partial x} \right\} \delta u(x, t).
\end{aligned} \tag{1.2.15}$$

Notice that the last explicit term in $\delta\mathcal{J}$ may be written as

$$2\int_0^T dt \int_0^L dx\, w \sum_{m=1}^{M} \{\hat{u}(x_m, t_m) - d_m\}\delta u(x,t)\delta(x - x_m)\delta(t - t_m), \tag{1.2.16}$$

where the second and third δs denote Dirac delta functions. We have now expressed $\delta\mathcal{J}$ entirely in terms of $\delta u(x,t)$. None of δu_t, δu_x and $\delta u(x_m, t_m)$ still appear.

We now argue that

$$\delta\mathcal{J} = O(\delta u)^2, \tag{1.2.17}$$

implying that $\hat{u}$ is an extremum of $\mathcal{J}$, provided that the coefficients of $\delta u(x,t)$, $\delta u(L,t)$, $\delta u(0,t)$, $\delta u(0,x)$ and $\delta u(T,x)$ all vanish. Examination of (1.2.12), (1.2.15) and (1.2.16) shows that these conditions are, respectively,

$$-\frac{\partial\lambda}{\partial t} - c\frac{\partial\lambda}{\partial x} + w\sum_{m=1}^{M}\{\hat{u}_m - d_m\}\delta(x - x_m)\delta(t - t_m) = 0, \tag{1.2.18}$$

$$\lambda(L,t) = 0, \tag{1.2.19}$$

$$-c\lambda(0,t) + W_b\{\hat{u}(0,t) - B(t)\} = 0, \tag{1.2.20}$$

$$-\lambda(x,0) + W_i\{\hat{u}(x,0) - I(x)\} = 0, \tag{1.2.21}$$

$$\lambda(x,T) = 0, \tag{1.2.22}$$

where $\hat{u}_m \equiv \hat{u}(x_m, t_m)$. Recall the definition of λ:

$$\lambda \equiv W_f\left\{\frac{\partial\hat{u}}{\partial t} + c\frac{\partial\hat{u}}{\partial x} - F\right\}. \tag{1.2.23}$$

These conditions (1.2.18)–(1.2.23) constitute the Euler–Lagrange equations for local extrema of the penalty functional $\mathcal{J}$ defined in (1.2.10). How shall we untangle them, to find our best-fit estimate $\hat{u}$ of the ocean circulation u?

Note 1. Substituting (1.2.23) into (1.2.18) yields "the" Euler–Lagrange equation familiar to physicists.

Note 2. Students sometimes derive (1.2.12) from (1.2.10) by expanding the squares in the integrand, evaluating at $\hat{u} + \delta u$ and at $\hat{u}$, and then subtracting. It is less tedious to calculate as follows:

$$\begin{aligned}\delta\mathcal{J}[u]\Big|_{u=\hat{u}} &= \delta W_f \int_0^T dt \int_0^L dx \left\{\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} - F\right\}^2 + \cdots \\ &= W_f \int_0^T dt \int_0^L dx\, \delta\left(\left\{\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} - F\right\}^2\right) + \cdots\end{aligned}$$

$$= W_f \int_0^T dt \int_0^L dx\, 2\left\{\frac{\partial \hat{u}}{\partial t} + c\frac{\partial \hat{u}}{\partial x} - F\right\}\delta\left\{\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} - F\right\} + \cdots$$

$$= 2W_f \int_0^T dt \int_0^L dx\left\{\frac{\partial \hat{u}}{\partial t} + c\frac{\partial \hat{u}}{\partial x} - F\right\}\left\{\frac{\partial \delta u}{\partial t} + c\frac{\partial \delta u}{\partial x}\right\} + \cdots, \tag{1.2.24}$$

as in (1.2.12).

Exercise 1.2.1 (requires care)
Consider the integral

$$\mathcal{I} = \int_0^T dt \int_0^L dx \lambda^2 . \tag{1.2.25}$$

Substitute for one of the factors of λ in (1.2.25), using (1.2.23). Integrate by parts, and use (1.2.18)–(1.2.22). Conclude that if W_f, W_b, W_i and $w > 0$, then the Euler–Lagrange equations (1.2.18)–(1.2.23) have a unique solution. Discuss the case $W_i = 0$; it occurs widely in the published literature (Bennett and Miller, 1991). □

Exercise 1.2.2
Consider slow, viscous flow driven by an externally imposed pressure gradient, as in Exercise 1.1.3. Assume measurements of u are available, as §1.2.2. Resolve this ill-posed problem by defining a generalized inverse in terms of a weighted, least-squares best fit to all the information. Derive the Euler–Lagrange equations, and prove that they have at most one solution. □

Exercise 1.2.3
Introduce a forcing error $\Delta t f_n^k$ into the finite-difference model (1.1.18). By analogy to (1.2.9), a simple penalty function is

$$J[u] = W_f \sum_k \sum_n \left(f_n^k\right)^2 \Delta x \Delta t + \cdots, \tag{1.2.26}$$

where the ellipsis indicates initial penalties, etc., that will be considered below in stages, as will the ranges of the summations in (1.2.26).

(i) Show that the Euler–Lagrange equation for extrema of J with respect to variations of u_n^k is

$$\lambda_n^{k-1} - \lambda_n^k - c(\Delta t/\Delta x)\left(\lambda_n^k - \lambda_{n+1}^k\right) = \cdots, \tag{1.2.27}$$

where the ellipses indicate contributions from variations of data penalties in (1.2.26).

(ii) The range of summation over the time index k in (1.2.26) is $0 \le k \le K-1$, where $K\Delta t = T$. By analogy to (1.2.9), a simple initial penalty is

$$J[u] = \cdots + W_i \sum_n \left(u_n^0 - I_n\right)^2 + \cdots . \tag{1.2.28}$$

Show that, for extrema with respect to u_n^0 and u_n^K,

$$-\lambda_n^0 + W_i \left\{\hat{u}_n^0 - I_n\right\} = 0 \tag{1.2.29}$$

and

$$\lambda_n^{K-1} = 0, \tag{1.2.30}$$

respectively. Compare these with (1.2.21) and (1.2.22).

(iii) Choose a range of summation over the space index n in (1.2.26), and prescribe a simple boundary penalty analogous to that in (1.2.9). Derive extremal conditions analogous to (1.2.19) and (1.2.20).

(iv) Assume that there are M measurements of u_n^k, that is, measured values of $u(x,t)$ at grid points in space and time. Prescribe a simple data penalty as in (1.2.9) and derive the contributions to (1.2.27) from variations of this data penalty.
Hint: Replace the Dirac delta functions $\delta(x_n - x_m)$ and $\delta(t_k - t_j)$ with $(\Delta x)^{-1}\delta_{nm}$ and $(\Delta t)^{-1}\delta_{kj}$ respectively, where δ_{nm} is the Kronecker delta:

$$\delta_{nm} = \begin{cases} 1 & n = m \\ 0 & n \neq m. \end{cases} \tag{1.2.31}$$

□

1.3 Solving the Euler–Lagrange equations using representers

1.3.1 Least-squares fitting by explicit solution of extremal conditions

The mixed initial-boundary value problem (1.1.1)–(1.1.3) for the first-order wave equation, together with the data (1.2.1) and the simple least-squares penalty functional (1.2.10), have led us to the awkward system of Euler–Lagrange equations (1.2.18)–(1.2.23). The solution is the best-fit ocean circulation $\hat{u}$. It may be obtained explicitly, by an intricate construction involving "representer functions". The effort is rewarded not only with structural insight, but also with enormous gains in computational efficiency compared to conventional minimization of (1.2.10) using gradient information.

1.3.2 The Euler–Lagrange equations are a two-point boundary value problem in time

After a little reordering, the Euler–Lagrange equations for local extrema $\hat{u}$ of the penalty functional $\mathcal{J}[u]$ are:

$$
(\mathrm{B})\begin{cases}
-\dfrac{\partial\lambda}{\partial t}-c\dfrac{\partial\lambda}{\partial x}=-w\displaystyle\sum_{m=1}^{M}\{\hat{u}_m-d_m\}\delta(x-x_m)\delta(t-t_m) & (1.3.1)\\
\lambda(x,T)=0 & (1.3.2)\\
\lambda(L,t)=0, & (1.3.3)
\end{cases}
$$

$$
(\mathrm{F})\begin{cases}
\dfrac{\partial\hat{u}}{\partial t}+c\dfrac{\partial\hat{u}}{\partial x}=F+W_f^{-1}\lambda & (1.3.4)\\
\hat{u}(x,0)=I(x)+W_i^{-1}\lambda(x,0) & (1.3.5)\\
\hat{u}(0,t)=B(t)+cW_b^{-1}\lambda(0,t). & (1.3.6)
\end{cases}
$$

Note 1. Our best estimates for f, i and b are

$$
\hat{f}(x,t)\equiv W_f^{-1}\lambda(x,t),\quad \hat{\imath}(x)\equiv W_i^{-1}\lambda(x,0),\quad \hat{b}(t)\equiv cW_b^{-1}\lambda(0,t). \tag{1.3.7}
$$

Note 2. Eq. (1.3.1) is known as the "backward" or "adjoint" equation.

Note 3. At first glance, it would seem that we could proceed by integrating the system (B) "backwards in time and to the left" (see Fig. 1.2.1), yielding $\hat{\lambda}(x,t)$, $\hat{\lambda}(0,t)$ and $\hat{\lambda}(x,0)$. Then we could integrate the system (F) "forwards and to the right" (see Fig. 1.2.1), yielding the ocean circulation estimate $\hat{u}=\hat{u}(x,t)$. However, after reexamining (1.3.1), we see that it is necessary to know $\hat{u}(x_m,t_m)$ in order to integrate (B). *The Euler–Lagrange equations do not consist of two initial-value problems; they comprise a single, two-point boundary value problem in the time interval* $0\le t\le T$.

1.3.3 Representer functions: the explicit solution and the reproducing kernel

Let us introduce the representer functions. There are M of them, denoted by $r_m(x,t)$, $1\le m\le M$. Each has an "adjoint" $\alpha_m(x,t)$, satisfying

$$
(\mathrm{B}_m)\begin{cases}
-\dfrac{\partial\alpha_m}{\partial t}-c\dfrac{\partial\alpha_m}{\partial x}=\delta(x-x_m)\delta(t-t_m) & (1.3.8)\\
\alpha_m(x,T)=0 & (1.3.9)\\
\alpha_m(L,t)=0. & (1.3.10)
\end{cases}
$$

As a consequence of the single impulse on the rhs of (1.3.8) being "bare", we may integrate (B_m) "backwards and to the left", yielding $\alpha_m(x,t)$. We may then solve for

r_m by integrating (F_m) "forward and to the right":

$$(\mathrm{F}_m)\begin{cases}\dfrac{\partial r_m}{\partial t}+c\dfrac{\partial r_m}{\partial x}=W_f^{-1}\alpha_m & (1.3.11)\\ r_m(x,0)=W_i^{-1}\alpha_m(x,0) & (1.3.12)\\ r_m(0,t)=cW_b^{-1}\alpha_m(0,t). & (1.3.13)\end{cases}$$

Next, we seek a solution of (1.3.1)–(1.3.6) in the form

$$\hat{u}(x,t)=u_F(x,t)+\sum_{m=1}^{M}\beta_m r_m(x,t), \tag{1.3.14}$$

where u_F is the prior estimate (the solution of the forward model (1.2.2)–(1.2.4)), and the β_m are unknown constants. If we substitute (1.3.14) into (1.3.4), and derive

$$D\hat{u}=Du_F+\sum_{m=1}^{M}\beta_m Dr_m \tag{1.3.15}$$

$$=F+W_f^{-1}\sum_{m=1}^{M}\beta_m\alpha_m, \tag{1.3.16}$$

where $D=\frac{\partial}{\partial t}+c\frac{\partial}{\partial x}$, we find that

$$\lambda\equiv W_f\{D\hat{u}-F\}=\sum_{m=1}^{M}\beta_m\alpha_m. \tag{1.3.17}$$

Furthermore,

$$\begin{aligned}-D\lambda&=-\sum_{m=1}^{M}\beta_m D\alpha_m\\ &=\sum_{m=1}^{M}\beta_m\delta(x-x_m)\delta(t-t_m) &(1.3.18)\\ &=-w\sum_{m=1}^{M}\{\hat{u}_m-d_m\}\delta(x-x_m)\delta(t-t_m), &(1.3.19)\end{aligned}$$

by virtue of (1.3.1). Equating coefficients of the impulses, we obtain the optimal choices $\hat{\beta}_m$ for the representer coefficients β_m:

$$\beta_m=\hat{\beta}_m\equiv-w\{\hat{u}_m-d_m\} \tag{1.3.20}$$

for $1\le m\le M$. Substituting again for $\hat{u}_m$ yields

$$\hat{\beta}_m=-w\left\{u_{F_m}+\sum_{l=1}^{M}\hat{\beta}_l r_{lm}-d_m\right\}, \tag{1.3.21}$$

where $u_{F_m}\equiv u_F(x_m,t_m)$ and $r_{lm}\equiv r_l(x_m,t_m)$.

Hence

$$\sum_{l=1}^{M}(r_{lm} + w^{-1}\delta_{lm})\hat{\beta}_l = h_m \equiv d_m - u_{F_m}, \tag{1.3.22}$$

where δ_{lm} is the Kronecker delta. In matrix notation, the M equations (1.3.22) for the M representer coefficients $\hat{\beta}_m$ become

$$(\mathbf{R} + w^{-1}\mathbf{I})\hat{\beta} = \mathbf{h} \equiv \mathbf{d} - \mathbf{u}_F. \tag{1.3.23}$$

Note 1. The rhs $\mathbf{h}$ is known; it is the data vector minus the vector of measured values of the prior estimate.

Note 2. The diagonal weight matrix $w\mathbf{I}$ is readily generalized to symmetric positive definite matrices $\mathbf{w}$.

Note 3. The l^{th} column of the $M \times M$ "representer matrix" $\mathbf{R}$ consists of the M measured values of the l^{th} representer function $r_l(x, t)$.

Note 4. It will be shown (see (1.3.32)) that $\mathbf{R}$ is symmetric: $\mathbf{R} = \mathbf{R}^{\mathrm{T}}$.

Note 5. The generalized inverse problem of finding the field $\hat{u} = \hat{u}(x, t)$, where $0 \le x \le L$ and $0 \le t \le T$, has been exactly reduced to the problem of inverting an $M \times M$ matrix, in order to find the M representer coefficients $\hat{\beta}$.

Finally, we have an explicit solution for $\hat{u}$:

$$\boxed{\hat{u}(x, t) = u_F(x, t) + (\mathbf{d} - \mathbf{u}_F)^{\mathrm{T}}(\mathbf{R} + \mathbf{w}^{-1})^{-1}\mathbf{r}(x, t).} \tag{1.3.24}$$

It was established in §1.1 that the forward model (1.1.1)–(1.1.3) has a unique solution for each choice of the inputs. Accordingly, the partial differential operator in (1.1.1), the initial operator in (1.1.2) and the boundary operator in (1.1.3) constitute a nonsingular operator. It may be inverted; the inverse operator is expressed explicitly in (1.1.17) with the Green's function γ. Introducing the measurement operators as in (1.2.1) yields a problem with no solution, thus the operator comprising those in (1.1.1)–(1.1.3) and (1.2.1) is singular; it is not invertible in the regular sense. However, a generalized inverse has been defined in the weighted least-squares sense of (1.2.10), and is explicitly expressed in (1.3.24) with the representers for the penalty functional (1.2.10), and with the Green's function for the nonsingular operator. Recall that u_F is given by (1.1.17), although it will in practice be computed by numerical integration of (1.2.2)–(1.2.4). In an abuse of language, we shall refer to the best-fit $\hat{u}$ given by (1.3.24) as the generalized inverse estimate, or simply the inverse.

Exercise 1.3.1

Verify that the initial condition (1.3.5) and boundary conditions (1.3.6) are satisfied. □

In summary, the steps for solving the Euler–Lagrange equations are:

(1) calculate $u_F(x,t)$ and hence $\mathbf{u}_F$;
(2) calculate $\mathrm{r}(x,t)$ and hence R;
(3) invert $\mathsf{P} \doteq \mathsf{R} + \mathsf{w}^{-1}$;
(4) assemble (1.3.24).

Note 1. $u_F(x,t)$ depends upon the "dynamics", the initial operator, the boundary operator and the choices for F, I and B.
Note 2. $\mathbf{u}_F$ depends upon u_F and the "observing network" $\{(x_m, t_m)\}_{m=1}^{M}$.
Note 3. $\mathbf{r}$ depends upon the dynamics, the initial operator, the boundary operator, the observing network and the inverted weights W_f^{-1}, W_i^{-1}, W_b^{-1}.
Note 4. $\hat{\boldsymbol{\beta}}$ depends upon R, the inverse of the data weight w, and the prior data misfit $\mathbf{h} \equiv \mathbf{d} - \mathbf{u}_F$.
Note 5. See Fig. 3.1.1 for a "time chart" implementing the representer solution.

Exercise 1.3.2
Express λ, $\hat{f}$, $\hat{\imath}$ and $\hat{b}$ using representer functions and their adjoints. □

Exercise 1.3.3 (trivial)
Show that

$$\mathcal{J}_F \equiv \mathcal{J}[u_F] = \mathbf{h}^{\mathrm{T}} \mathsf{w}\, \mathbf{h}. \tag{1.3.25}$$

□

Exercise 1.3.4 (nontrivial)
Show that

$$\text{(i)} \quad \hat{\mathcal{J}} \equiv \mathcal{J}[\hat{u}] = \mathbf{h}^{\mathrm{T}} \mathsf{P}^{-1} \mathbf{h}, \tag{1.3.26}$$

$$\text{(ii)} \quad \hat{\mathcal{J}}_{\text{data}} \equiv (\mathbf{d} - \hat{\mathbf{u}})^{\mathrm{T}} \mathsf{w} (\mathbf{d} - \hat{\mathbf{u}}) = \mathbf{h}^{\mathrm{T}} \mathsf{P}^{-1} \mathsf{w}^{-1} \mathsf{P}^{-1} \mathbf{h}, \tag{1.3.27}$$

and

$$\text{(iii)} \quad \hat{\mathcal{J}}_{\text{mod}} \equiv \hat{\mathcal{J}} - \hat{\mathcal{J}}_{\text{data}} = \mathbf{h} \mathsf{P}^{-1} \mathsf{R} \mathsf{P}^{-1} \mathbf{h}. \tag{1.3.28}$$

Note that $\hat{\mathcal{J}}_{\text{mod}}$ is the sum of dynamical, initial and boundary penalties. □

Let us now prove that the representer matrix is symmetric: $\mathsf{R} = \mathsf{R}^{\mathrm{T}}$.

First, recall that the adjoint representer $\alpha_m(x,t)$ for a point measurement at (x_m, t_m) is just the Green's function $\gamma(x, t, x_m, t_m)$, where $\gamma(x, t, y, s)$ satisfies

$$-\frac{\partial \gamma}{\partial t} - c\frac{\partial \gamma}{\partial x} = \delta(x - y)\delta(t - s), \tag{1.3.29}$$

subject to $\gamma = 0$ at $t = T$, $\gamma = 0$ at $x = L$. Now let $\Gamma(x, t, y, s)$ satisfy

$$\frac{\partial}{\partial t}\Gamma + c\frac{\partial}{\partial x}\Gamma = W_f^{-1}\gamma, \tag{1.3.30}$$

subject to $\Gamma = W_i^{-1}\gamma$ at $t = 0$, and $\Gamma = cW_b^{-1}\gamma$ at $x = 0$. Thus $r_m(x, t) = \Gamma(x, t, x_m, t_m)$.

Exercise 1.3.5 (Bennett, 1992)
Show that

$$\begin{aligned}\Gamma(x, t, y, s) = W_f^{-1}\int dz \int dr\, \gamma(z, r, x, t)\gamma(z, r, y, s)\\ + W_i^{-1}\int dz\, \gamma(z, 0, x, t)\gamma(z, 0, y, s)\\ + c^2 W_b^{-1}\int dr\, \gamma(0, r, x, t)\gamma(0, r, y, s).\end{aligned} \tag{1.3.31}$$

Hence representers are not Green's functions; rather they are "squares" of Green's functions. Note that Γ is symmetric, but γ is *not* symmetric. □

Finally we deduce that

$$\begin{aligned} r_{lm} \equiv r_l(x_m, t_m) &= \Gamma(x_m, t_m, x_l, t_l)\\ &= \Gamma(x_l, t_l, x_m, t_m)\\ &= r_m(x_l, t_l)\\ &\equiv r_{ml}. \end{aligned} \tag{1.3.32}$$

That is, $\mathbf{R} = \mathbf{R}^{\mathrm{T}}$. Note that Γ is known as a "reproducing kernel" or "rk", for reasons given in §2.1.

1.4 Some limiting choices of weights: "weak" and "strong" constraints

1.4.1 Diagonal data weight matrices, for simplicity

The parade of formulae in the previous sections should become more meaningful as we explore some limiting choices for the weights. We shall assume that the data weight matrix is diagonal:

$$\mathbf{w} = w\mathbf{I}, \tag{1.4.1}$$

in order to avoid technicalities such as the norm of a matrix. Note that (1.4.1) implies

$$\mathbf{w}^{-1} = w^{-1}\mathbf{I}. \tag{1.4.2}$$

1.4.2 Perfect data

If we believe that the data are perfectly accurate, then we should give infinite weight to them. In this case we hope that the inverse estimates agree exactly with the data, at the measurement sites. Let us therefore consider the limit: $w \to \infty$.

Hence

$$\mathbf{P} \equiv \mathbf{R} + w^{-1}\mathbf{I} \to \mathbf{R}, \tag{1.4.3}$$

$$\hat{\boldsymbol{\beta}} \to \mathbf{R}^{-1}\mathbf{h}, \tag{1.4.4}$$

and

$$\hat{u}(x,t) \to u_F(x,t) + \mathbf{r}(x,t)^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{h}. \tag{1.4.5}$$

Measuring both sides of (1.4.5) yields

$$\hat{\mathbf{u}} \to \mathbf{u}_F + \mathbf{R}^{\mathrm{T}}\mathbf{R}^{-1}\mathbf{h}, \tag{1.4.6}$$

$$= \mathbf{u}_F + \mathbf{h} \tag{1.4.7}$$

$$= \mathbf{u}_F + (\mathbf{d} - \mathbf{u}_F) \tag{1.4.8}$$

$$= \mathbf{d}, \tag{1.4.9}$$

as required. Note that we have used the symmetry of the representer matrix: $\mathbf{R}^{\mathrm{T}} = \mathbf{R}$. In this limit, the inverse estimate *interpolates* the data.

1.4.3 Worthless data

Now suppose that we believe the data are worthless, that is, we have no information about the magnitude of the data errors. In practice we always have some idea: the errors in altimetry data do not exceed the height of the orbit of the satellite, but that is infinite by any hydrographic standard. We should therefore consider the limit: $w \to 0$. Then

$$\mathbf{P}^{-1} = (\mathbf{R} + w^{-1}\mathbf{I})^{-1} \to \mathbf{0}, \tag{1.4.10}$$

hence

$$\hat{u}(x,t) \to u_F(x,t). \tag{1.4.11}$$

That is, the data have no influence on the inverse estimate, as would be desirable.

1.4.4 Rescaling the penalty functional

The Euler–Lagrange equations for local extrema of $\mathcal{J}[u]$ are also those for local extrema of $2\mathcal{J}[u]$. This is true even if the dynamics and observing systems are nonlinear, or if $\mathcal{J}$ is not quadratic. Thus the limiting cases: $w \to \infty$, $w \to 0$ really refer to w/W_f, w/W_i, w/W_b all $\to \infty$, or all $\to 0$. That is, they refer to the relative weighting of the various information. However, the prior and posterior functional values $\mathcal{J}_F \equiv \mathcal{J}[u_F]$, and $\hat{\mathcal{J}} \equiv \mathcal{J}[\hat{u}]$ do depend upon the absolute values of the weights. This will be crucial later, when we interpret these numbers as test statistics for the model as a formal hypothesis about the ocean.

1.4.5 Perfect dynamics: Lagrange multipliers for strong constraints

The admission of the error field $f = f(x,t)$ in (1.2.6), and the inclusion of $W_f \int_0^L dx \int_0^T dt\, f^2$ in the penalty functional (1.2.9), leads to the model being described as a "weak constraint" upon the inversion process (Sasaki, 1970). The model may alternatively be imposed as a "strong constraint". In that case, the penalty functional is

$$\mathcal{K}[u] = W_i \int_0^L dx\, i(x)^2 + W_b \int dt\, b(t)^2 + w \sum_{m=1}^{M} \epsilon_m^2 . \tag{1.4.12}$$

Compare (1.4.12) and (1.2.9): i, b and ϵ_m are defined as before by (1.2.7), (1.2.8) and (1.2.1) respectively, but now we require that $u = u(x,t)$ satisfy (1.1.1) exactly. This requirement may be met in the search for the minimum of $\mathcal{K}$, by appending the strong constraint (1.1.1) to $\mathcal{K}$ using a Lagrange multiplier field $\psi = \psi(x,t)$:

$$\mathcal{L}[u,\psi] = \mathcal{K}[u] + 2\int_0^L dx \int_0^T dt\, \psi(x,t) \left\{ \frac{\partial u}{\partial t}(x,t) + c\frac{\partial u}{\partial x}(x,t) - F(x,t) \right\}. \tag{1.4.13}$$

The factor of two will be seen to be convenient. Note that the augmented penalty functional $\mathcal{L}$ depends on u and ψ, which may vary independently. The total variation in $\mathcal{L}$ is

$$\begin{aligned} \delta\mathcal{L} = \delta\mathcal{K} &+ 2\int_0^L dx \int_0^T dt\, \delta\psi \left(\frac{\partial u}{\partial t} + c\frac{\partial u}{\partial x} - F \right) \\ &+ 2\int_0^L dx \int_0^T dt\, \psi \left(\delta\frac{\partial u}{\partial t} + c\delta\frac{\partial u}{\partial x} \right) + O(\delta^2). \end{aligned} \tag{1.4.14}$$

If the pair of fields $\hat{\psi} = \hat{\psi}(x,t)$ and $\hat{u} = \hat{u}(x,t)$ extremize $\mathcal{L}$ for arbitrary variations $\delta\psi$ and δu, then

$$-\frac{\partial \psi}{\partial t} - c\frac{\partial \psi}{\partial x} = -w\sum_{m=1}^{M} \{\hat{u}_m - d_m\}\,\delta(x - x_m)\delta(t - t_m) \tag{1.4.15}$$

$$\psi(x,T) = 0 \tag{1.4.16}$$

$$\psi(L,t) = 0 \tag{1.4.17}$$

$$\frac{\partial \hat{u}}{\partial t} + c\frac{\partial \hat{u}}{\partial x} = F \tag{1.4.18}$$

$$\hat{u}(x,0) = I(x) + W_i^{-1}\psi(x,0) \tag{1.4.19}$$

$$\hat{u}(0,t) = B(t) + cW_b^{-1}\psi(0,t). \tag{1.4.20}$$

The strong constraint (1.4.18) is immediately recovered from (1.4.14), if $\delta\mathcal{L}=0$ and $\delta\psi$ is arbitrary. The other Euler–Lagrange conditions are recovered as in §1.2. Comparing (1.4.15)–(1.4.20) with (1.3.1)–(1.3.6) establishes that

$$\psi(x,t)=\lim_{W_f\to\infty}\lambda(x,t)\,. \tag{1.4.21}$$

It would seem from (1.3.1)–(1.3.3) that λ is independent of W_f, but there is an implicit dependence through $\hat{u}_m$, $1\le m\le M$, in (1.3.1). Thus, we may recover the "strong constraint" inverse from the "weak constraint" inverse in the limit as $W_f\to\infty$.

1.5 Regularity of the inverse estimate

1.5.1 Physical realizability

Thus far our construction has been formal: we paid no attention to the physical realizability of the inverse estimate $\hat{u}$. We shall now see that $\hat{u}$ is in fact unrealistic, unless we make more interesting choices for the weights W_f, W_i and W_b.

1.5.2 Regularity of the Green's functions and the adjoint representer functions

Consider "the" Euler–Lagrange equation:

$$-\frac{\partial\lambda}{\partial t}-c\frac{\partial\lambda}{\partial x}=-w\sum_{m=1}^{M}(d_m-\hat{u}_m)\delta(x-x_m)\delta(t-t_m). \tag{1.5.1}$$

In fact, just consider the equation for an adjoint representer function:

$$-\frac{\partial\alpha_m}{\partial t}-c\frac{\partial\alpha_m}{\partial x}=\delta(x-x_m)\delta(t-t_m), \tag{1.5.2}$$

subject to

$$\alpha_m(x,T)=0,\quad \alpha_m(L,t)=0\,. \tag{1.5.3}$$

The solution is the Green's function:

$$\begin{aligned}\alpha_m(x,t)&=\gamma(x,t,x_m,t_m)\\&=\delta(x-x_m-c(t-t_m))H(t_m-t),\end{aligned} \tag{1.5.4}$$

and $\lambda(x,t)=\beta^{\mathrm{T}}\alpha(x,t)$. Clearly the α_m and hence λ are singular, and not just at the data points $(x_m,\ t_m)$: see Fig. 1.5.1.

Now $\hat{u}$ obeys

$$\frac{\partial\hat{u}}{\partial t}+c\frac{\partial\hat{u}}{\partial x}=F+\hat{f}=F+W_f^{-1}\lambda, \tag{1.5.5}$$

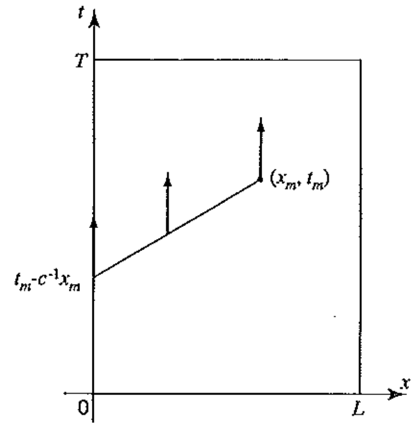

Figure 1.5.1 Support of $\alpha_m(x, t)$. The arrows (the delta functions) are normal to the page.

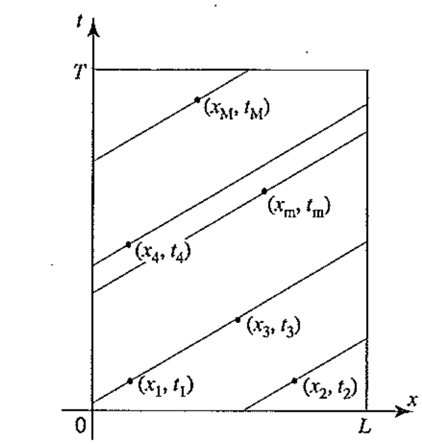

Figure 1.5.2 Support of singularities in $\hat{u}(x, t)$.

subject to the initial and boundary conditions

$$\hat{u} = I + \hat{\imath} = I + W_i^{-1}\lambda, \quad \hat{u} = B + \hat{b} = B + cW_b^{-1}\lambda\,. \qquad (1.5.6)$$

So our estimates of $\hat{f}$, $\hat{\imath}$ and $\hat{b}$ are singular. There is neither dispersion nor diffusion in our "toy" ocean dynamics, so $\hat{u}$ is also singular: see Fig. 1.5.2. This is hardly a satisfactory combination of dynamics and data!

Exercise 1.5.1

Express r_m and $\hat{u}$ using the Green's function γ. □

1.5.3 Nondiagonal weighting: kernel inverses of weights

We want the data to influence the circulation at remote places and times, so we should give weight to products of residuals at remote places and times. We therefore generalize the penalty functional (1.2.9) to

$$\mathcal{J}[u] = \int_0^T dt \int_0^T ds \int_0^L dx \int_0^L dy\, f(x,t) W_f(x,t,y,s) f(y,s)$$

$$+ \int_0^L dx \int_0^L dy\, i(x) W_i(x,y) i(y) + \int_0^T dt \int_0^T ds\, b(t) W_b(t,s) b(s)$$

$$+ \sum_{l=1}^{M} \sum_{m=1}^{M} \epsilon_l w_{lm} \epsilon_m. \tag{1.5.7}$$

Thus our previous, trivial choices were

$$W_f(x,t,y,s) = W_f \cdot \delta(x-y)\delta(t-s), \quad \text{etc.} \tag{1.5.8}$$

The notations

$$\bullet \equiv \int_0^T dt \int_0^L dx, \quad \circ \equiv \int_0^L dx, \quad * \equiv \int_0^T dt$$

allow us to write $\mathcal{J}$ more compactly as

$$\mathcal{J}[u] = f \bullet W_f \bullet f + i \circ W_i \circ i + b * W_b * b + \epsilon^{\mathrm{T}} \mathbf{w} \epsilon. \tag{1.5.9}$$

Exercise 1.5.2

Define the weighted residual or adjoint variable $\lambda(x,t)$ by

$$\lambda \equiv W_f \bullet \left\{ \frac{\partial \hat{u}}{\partial t} + c \frac{\partial \hat{u}}{\partial x} - F \right\}. \tag{1.5.10}$$

Then show that the Euler–Lagrange equations for minima of (1.5.9) are just as before. □

Exercise 1.5.3

Define C_f, the inverse of W_f, by

$$C_f \bullet W_f \equiv \int_0^T dr \int_0^L dz\, C_f(x,t,z,r) W_f(z,r,y,s) \tag{1.5.11}$$

$$= \delta(x-y)\delta(t-s). \tag{1.5.12}$$

Define C_i and C_b analogously, and define $\mathbf{C}_\epsilon$ by

$$\mathbf{w}\mathbf{C}_\epsilon = \mathbf{I}. \tag{1.5.13}$$

Each entity in (1.5.13) is an $M \times M$ matrix. Now, write out the representer solution of the Euler–Lagrange equations. Verify that the solution only requires C_f, C_i, C_b and $\mathbf{C}_\epsilon$; that is, it does not require their inverses, the weights W_f, W_i, W_b and $\mathbf{w}$. □

1.5.4 The inverse weights smooth the residuals

The inverse estimate $\hat{u}$ obeys

$$\frac{\partial \hat{u}}{\partial t}(x,t) + c\frac{\partial \hat{u}}{\partial x}(x,t) = F(x,t) + (C_f \bullet \lambda)(x,t)$$
$$= F(x,t) + \int_0^T ds \int_0^L dy\, C_f(x,t,y,s)\lambda(y,s), \quad (1.5.14)$$

subject to

$$\hat{u}(x,0) = I(x) + (C_i \circ \lambda)(x,0), \quad (1.5.15)$$

and

$$\hat{u}(0,t) = B(t) + c(C_b * \lambda)(0,t). \quad (1.5.16)$$

The supposition is that C_f, C_i and C_b smooth the singular behavior of λ, yielding regular estimates for $\hat{f} \equiv C_f \bullet \lambda$, $\hat{\imath} \equiv C_i \circ \lambda$ and $\hat{b} = cC_b * \lambda$, leading in turn to a regular estimate $\hat{u}$ for the ocean circulation.

In summary, we should avoid "diagonal" weighting.

Note 1. The adjoint variables α and λ remain singular, but $\mathbf{r}$ and u should become regular.

Note 2. Evaluation of the convolutions in (1.5.14), (1.5.15) and (1.5.16) at each position and time is potentially very expensive: consider *three* space dimensions and time.

Note 3. Functional analysis sheds much light on smoothness: see §2.6.

Exercise 1.5.4

Consider slow, viscous flow as discussed in Exercises 1.1.3 and 1.2.2. Construct both the adjoint representers α and the representers $\mathbf{r}$, using the Green's function ϕ given in (1.1.26). How smooth are α and $\mathbf{r}$? Is nondiagonal weighting of either the dynamical penalty or the initial penalty necessary? □

Exercise 1.5.5

Generalize the definition of the rk Γ given in (1.3.30) *et seq.* Prove that

(i) $r_m(x,t) = \Gamma(x,t,x_m,t_m)$, (1.5.17)
for $1 \le m \le M$;

(ii) $\Gamma = \gamma \bullet C_f \bullet \gamma + \gamma \circ C_i \circ \gamma + c^2 \gamma * C_b * \gamma$. (1.5.18)

□

Note:
The adjoint equations (1.3.1)–(1.3.3) and forward equations (1.5.14)–(1.5.16), which constitute the most general form of the Euler–Lagrange equations developed in §1.2 and §1.5, are restated for convenience in §4.2 as (4.2.1)–(4.2.6).