5

Variational inverse problems

The purpose of this chapter is to introduce the basic formalism needed for properly formulating and solving linear variational inverse problems. Contrary to the sequential methods which update the model solution every time observations are available, variational methods seek an estimate in space and time where the estimate at a particular time is dependent on both past and future measurements.

We start by discussing a very simple example to illustrate the inverse problem and in particular the effect of including model errors. Thereafter a simple scalar model is used in a more typical illustration where the general formulation of the inverse problem is discussed and the Euler–Lagrange equations which determine the minimizing solution are derived.

Different methods are available for solving the Euler–Lagrange equations and we briefly discuss the popular representer method (see *Bennett*, 1992, 2002) which has proven extremely useful for solving linear and weakly nonlinear variational inverse problems.

5.1 Simple illustration

We will start with a very simple example to illustrate the mathematical properties of a variational problem and the difference between a weak and a strong constraint formulation. We define the simple model

$$\frac{d\psi}{dt} = 1, \tag{5.1}$$

$$\psi(0) = 0, \tag{5.2}$$

$$\psi(1) = 2, \tag{5.3}$$

having one initial condition and one final condition. Clearly this is an overdetermined problem and it has no solution. However, if we relax the conditions by adding unknown errors to each of them the system becomes

$$\frac{d\psi}{dt} = 1 + q, \tag{5.4}$$
$$\psi(0) = 0 + a, \tag{5.5}$$
$$\psi(1) = 2 + b. \tag{5.6}$$

The system is now under-determined since we can get whatever solution we want by choosing the different error terms. A statistical hypothesis $\mathcal{H}_0$, is now needed for the error terms,

$$\begin{aligned}
\overline{q(t)} &= 0, & \overline{q(t_1)q(t_2)} &= C_0\delta(t_1 - t_2), & \overline{q(t)a} &= 0, \\
\overline{a} &= 0, & \overline{a^2} &= C_0, & \overline{ab} &= 0, \\
\overline{b} &= 0, & \overline{b^2} &= C_0, & \overline{q(t)b} &= 0.
\end{aligned} \tag{5.7}$$

That is, we assume that we know the statistical behaviour of the error terms through their first and second order moments. In this example the variances are all set equal to C_0 for simplicity.

It is now possible to seek the solution, which is as close as possible to the initial and final conditions while at the same time it almost satisfies the model equations, by minimizing the error terms in the form of a weak constraint penalty function

$$\mathcal{J}[\psi] = W_0 \int_0^1 \left(\frac{d\psi}{dt} - 1 \right)^2 dt + W_0 \big(\psi(0) - 0\big)^2 + W_0 \big(\psi(1) - 2\big)^2, \tag{5.8}$$

where W_0 is the inverse of the error variance C_0. Then ψ is an extremum of the penalty function if

$$\delta\mathcal{J}[\psi] = \mathcal{J}[\psi + \delta\psi] - \mathcal{J}[\psi] = \mathcal{O}\big(\delta\psi^2\big), \tag{5.9}$$

when $\delta\psi \to 0$. Now, using

$$\begin{aligned}
\mathcal{J}[\psi + \delta\psi] = W_0 \int_0^1 & \left(\frac{d\psi}{dt} - 1 + \frac{d\delta\psi}{dt} \right)^2 dt \\
& + W_0 \big(\psi(0) - 0 + \delta\psi(0)\big)^2 + W_0 \big(\psi(1) - 2 + \delta\psi(1)\big)^2
\end{aligned} \tag{5.10}$$

in (5.9) and dropping the common nonzero factor $2W_0$, and all terms proportional to $\mathcal{O}\big(\delta\psi^2\big)$, we must have

$$\int_0^1 \frac{d\delta\psi}{dt} \left(\frac{d\psi}{dt} - 1 \right) dt + \delta\psi(0)\big(\psi(0) - 0\big) + \delta\psi(1)\big(\psi(1) - 2\big) = 0, \tag{5.11}$$

or from integration by part,

$$\begin{aligned}
\delta\psi & \left(\frac{d\psi}{dt} - 1 \right) \Bigg|_0^1 - \int_0^1 \delta\psi \frac{d^2\psi}{dt^2} dt \\
& + \delta\psi(0)\big(\psi(0) - 0\big) + \delta\psi(1)\big(\psi(1) - 2\big) = 0.
\end{aligned} \tag{5.12}$$

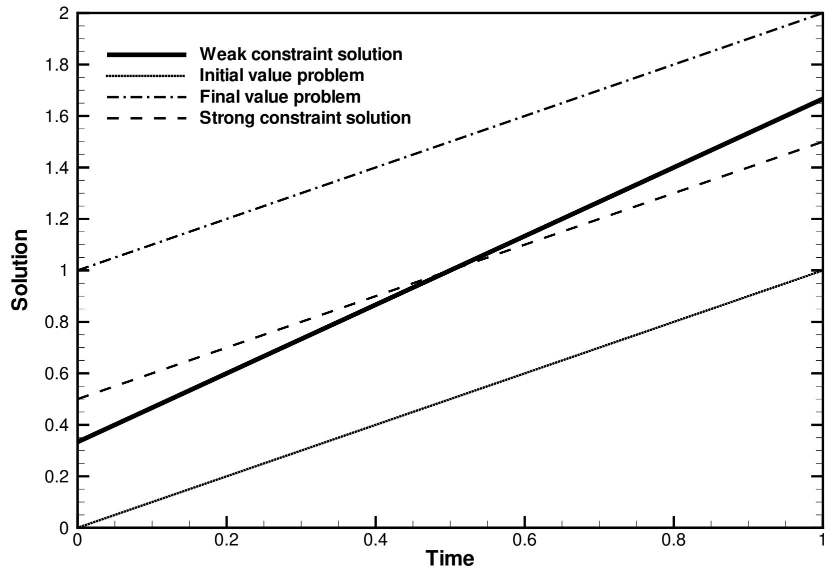

Fig. 5.1. Inverse solution from the simple example

This gives the following system of equations

$$\delta\psi(0)\left(-\frac{d\psi}{dt}+1+\psi\right)\bigg|_{t=0}=0, \tag{5.13}$$

$$\delta\psi(1)\left(\frac{d\psi}{dt}-1+\psi-2\right)\bigg|_{t=1}=0, \tag{5.14}$$

$$\delta\psi\left(\frac{d^2\psi}{dt^2}\right)=0, \tag{5.15}$$

or since $\delta\psi$ is arbitrary

$$\frac{d\psi}{dt}-\psi=1 \qquad \text{for } t=0, \tag{5.16}$$

$$\frac{d\psi}{dt}+\psi=3 \qquad \text{for } t=1, \tag{5.17}$$

$$\frac{d^2\psi}{dt^2}=0. \tag{5.18}$$

This is an elliptic boundary value problem in time with mixed Dirichlet and Neumann boundary conditions. The general solution is

$$\psi=c_1t+c_2, \tag{5.19}$$

and the constants in this case become $c_1=4/3$ and $c_2=1/3$.

In the case when we let the errors in the dynamical model go to zero, we approach the strong constraint limit where the dynamical model is assumed to be perfect. The strong constraint model solution is $\psi = t + c_2$ from (5.4), i.e. the slope is the one defined by the original model and no deviation of this is allowed. The free constant c_2 will take a value between 0 and 1, depending on the relative magnitude between the weights on the two conditions. In this case with equal weight we will have $c_2 = 0.5$.

By allowing for model errors to account for an imperfect model, we will through a weak constraint variational formulation also allow for a deviation from the exact model trajectory. This is important for the mathematical conditioning of the variational problem, and we will later see that the weak constraint problem can be solved as easily as the strong constraint problem. The results from this example are shown in Fig. 5.1. The upper and lower curves are the respective solutions of the final and initial value problems. The weak constraint inverse estimate is seen to have a steeper slope than the exact model would allow, in order to obtain an estimate in better agreement with the two conditions. The strong constraint estimate is shown for comparison.

Finally, it is interesting to examine what the KF solution becomes in this example. The KF starts by solving the initial value problem until $t = 1$, thus for $t \in [0, 1)$ the solution is just $\psi(t) = t$. The initial error variance is set to C_0 and the increase of error variance when integrating the model over one time unit is also C_0. Thus for the prediction at $t = 1$, the error variance equals $2C_0$. The update equation (3.14) then becomes

$$\begin{aligned}
\psi^{\mathrm{a}} &= \psi^{\mathrm{f}} + \frac{C^{\mathrm{f}}_{\psi\psi}}{C_{\epsilon\epsilon} + C^{\mathrm{f}}_{\psi\psi}} \left(d - \psi^{\mathrm{f}} \right) \\
&= 1 + \frac{2C_0}{C_0 + 2C_0} (2 - 1) \\
&= 5/3.
\end{aligned} \tag{5.20}$$

This is in fact identical to the weak constraint variational solution at $t = 1$. Thus, could there be some connection between the problem solved by a variational method and the KF? In fact it will be shown later that for linear inverse problems, the KF and the weak constraint variational method, when both formulated consistently and using the same prior error statistics, give identical solutions at the final time. Thus for forecasting purposes, it does not matter which method is used.

5.2 Linear inverse problem

In this section we will define the inverse problem for a simple linear model and derive the Euler–Lagrange equations for a weak constraint variational formulation.