

The Euler-Lagrange Equations

This section teaches us formally about the variational procedure of describing an inverse problem, backward (or adjoint) variables and the strong and weak constraint formulations. The method of representers, used to solve the Euler-Lagrange equations, is also introduced.

Statement of problem

What is the optimal state, $\phi(x, t)$ of the 1-D system whose dynamics are governed by

$$\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} - F = e, \quad (1)$$

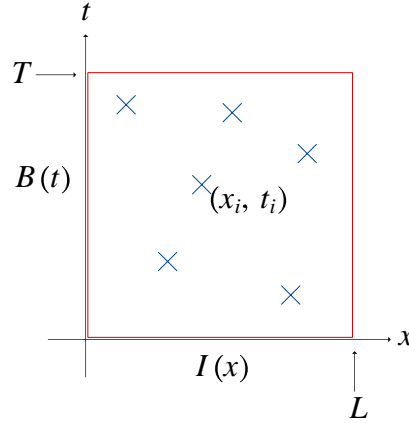
which lies close to given observations, initial conditions and boundary conditions?

ϕ : unknown tracer concentration, u : known constant advection speed, F : known source field, e : unknown model error.

Imperfectly known initial conditions (i.c.): $\phi(x, 0) \approx I(x)$, $0 \leq x \leq L$.

Imperfectly known boundary conditions (b.c.): $\phi(0, t) \approx B(t)$, $0 \leq t \leq T$.

Imperfect observation of the system: y_m (a direct observation of $\phi(x_m, t_m)$), $1 \leq m \leq M$.



Error standard deviations:

A-priori i.c.: $W_{ic}^{-1/2}$, a-priori b.c.: $W_{bc}^{-1/2}$, obs: $W_{ob}^{-1/2}$, model error $W_e^{-1/2}$.

The a-priori state $\phi_B(x, t)$:

$$\frac{\partial \phi_B}{\partial t} + u \frac{\partial \phi_B}{\partial x} - F = 0, \quad \phi_B(x, 0) = I(x), \quad \phi_B(0, t) = B(t). \quad (2, 3, 4)$$

I: The strong constraint formulation

Construct a functional $f[\phi]$:

$$f[\phi] = W_{ic} \int_{x=0}^L dx \{ \phi(x, 0) - I(x) \}^2 + W_{bc} \int_{t=0}^T dt \{ \phi(0, t) - B(t) \}^2 + W_{ob} \sum_{i=1}^M \{ \phi(x_i, t_i) - y_i \}^2. \quad (5)$$

What $\phi(x, t)$ makes $f[\phi]$ stationary, subject to the following model constraint?

$$g(x, t) = \frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} - F = 0. \quad (6)$$

The constrained minimization problem:

$$\begin{aligned}
J[\phi, \lambda] &= f[\phi] + 2 \int_{x=0}^L dx \int_{t=0}^T dt \lambda(x, t) g(x, t), \\
&= W_{ic} \int_{x=0}^L dx \{\phi(x, 0) - I(x)\}^2 + W_{bc} \int_{t=0}^T dt \{\phi(0, t) - B(t)\}^2 + \\
&\quad W_{ob} \sum_{i=1}^M \{\phi(x_i, t_i) - y_i\}^2 + 2 \int_{x=0}^L dx \int_{t=0}^T dt \lambda(x, t) \left(\frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} - F \right). \quad (7)
\end{aligned}$$

Minimize (7) w.r.t. the fields $\phi(x, t)$ and $\lambda(x, t)$. (5, 6) comprise a constrained minimization problem w.r.t. ϕ ; (7) comprises an unconstrained minimization problem w.r.t. ϕ and λ .

Construct variations of J about the reference fields $\hat{\phi}, \hat{\lambda}$, i.e.

$$J[\hat{\phi} + \delta\phi, \hat{\lambda} + \delta\lambda] = J[\hat{\phi}, \hat{\lambda}] + \delta J|_{\hat{\phi}, \hat{\lambda}}, \quad (8)$$

$$\delta J|_{\hat{\phi}, \hat{\lambda}} = \int_{x=0}^L dx \int_{t=0}^T dt \left. \frac{\partial J}{\partial \phi} \right|_{\hat{\phi}, \hat{\lambda}} \delta\phi + \int_{x=0}^L dx \int_{t=0}^T dt \left. \frac{\partial J}{\partial \lambda} \right|_{\hat{\phi}, \hat{\lambda}} \delta\lambda + O(\delta\phi^2, \delta\lambda^2, \delta\phi\delta\lambda), \quad (9)$$

$$\begin{aligned}
&= 2W_{ic} \int_{x=0}^L dx \{\hat{\phi}(x, 0) - I(x)\} \delta\phi(x, 0) + \\
&\quad 2W_{bc} \int_{t=0}^T dt \{\hat{\phi}(0, t) - B(t)\} \delta\phi(0, t) + \\
&\quad 2W_{ob} \sum_{i=1}^M \{\hat{\phi}(x_i, t_i) - y_i\} \delta\phi(x_i, t_i) + \\
&\quad 2 \int_{x=0}^L dx \int_{t=0}^T dt \hat{\lambda}(x, t) \left(\frac{\partial \delta\phi}{\partial t} + u \frac{\partial \delta\phi}{\partial x} \right) + \quad (*) \\
&\quad 2 \int_{x=0}^L dx \int_{t=0}^T dt \delta\lambda(x, t) \left(\frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} - F \right) + \\
&\quad O(\delta\phi^2, \delta\lambda^2, \delta\phi\delta\lambda). \quad (10)
\end{aligned}$$

Conditions on $\hat{\lambda}$: $\hat{\lambda}(x, T) = 0$, $\hat{\lambda}(L, t) = 0$.

The term marked (*) in (10) is not in the required form. Use the integration by parts formula to rewrite

$$" \int_a^b v \frac{du}{dx} dx = [uv]_a^b - \int_a^b u \frac{dv}{dx} dx ". \quad (11)$$

The first term in (*):

$$\begin{aligned}
\int_{t=0}^T dt \hat{\lambda}(x, t) \frac{\partial \delta\phi}{\partial t} &= [\delta\phi \hat{\lambda}]_0^T - \int_{t=0}^T dt \delta\phi \frac{\partial \hat{\lambda}}{\partial t}, \\
&= \delta\phi(x, T) \hat{\lambda}(x, T) - \delta\phi(x, 0) \hat{\lambda}(x, 0) - \int_{t=0}^T dt \delta\phi \frac{\partial \hat{\lambda}}{\partial t}. \quad (12)
\end{aligned}$$

The second term in (*):

$$\begin{aligned} \int_{x=0}^L dx \hat{\lambda}(x, t) u \frac{\partial \delta \phi}{\partial x} &= u [\delta \phi \hat{\lambda}]_0^L - \int_{x=0}^L dx u \delta \phi \frac{\partial \hat{\lambda}}{\partial x}, \\ &= u \delta \phi(L, t) \hat{\lambda}(L, t) - u \delta \phi(0, t) \hat{\lambda}(0, t) - \int_{x=0}^L dx u \delta \phi \frac{\partial \hat{\lambda}}{\partial x}. \end{aligned} \quad (13)$$

Note also for the observation term:

$$\{\hat{\phi}(x_i, t_i) - y_i\} \delta \phi(x_i, t_i) = \int_{x=0}^L dx \int_{t=0}^T dt \{\hat{\phi}(x_i, t_i) - y_i\} \delta \phi(x, t) \delta(x - x_i) \delta(t - t_i). \quad (14)$$

Using (12), (13) and (14) in (10) and noting the conditions on $\hat{\lambda}$:

$$\begin{aligned} \delta J \Big|_{\hat{\phi}, \hat{\lambda}} &= 2W_{ic} \int_{x=0}^L dx \{\hat{\phi}(x, 0) - I(x)\} \delta \phi(x, 0) + 2W_{bc} \int_{t=0}^T dt \{\hat{\phi}(0, t) - B(t)\} \delta \phi(0, t) + \\ &2W_{ob} \int_{x=0}^L dx \int_{t=0}^T dt \sum_{i=1}^M \{\hat{\phi}(x_i, t_i) - y_i\} \delta \phi(x, t) \delta(x - x_i) \delta(t - t_i) - \\ &2 \int_{x=0}^L dx \hat{\lambda}(x, 0) \delta \phi(x, 0) - 2 \int_{x=0}^L dx \int_{t=0}^T dt \frac{\partial \hat{\lambda}}{\partial t} \delta \phi(x, t) - \\ &2 \int_{t=0}^T dt u \hat{\lambda}(0, t) \delta \phi(0, t) - 2 \int_{t=0}^T dt \int_{x=0}^L dx u \frac{\partial \hat{\lambda}}{\partial x} \delta \phi(x, t) + \\ &2 \int_{x=0}^L dx \int_{t=0}^T dt \left(\frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} - F \right) \delta \lambda(x, t) + O(\delta \phi^2, \delta \lambda^2, \delta \phi \delta \lambda). \end{aligned} \quad (15)$$

Setting the linear part of (15) to zero, and using the conditions on $\hat{\lambda}$, gives Euler-Lagrange equations for the strong constraint:

$$\frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} - F = 0, \quad (16)$$

$$W_{ic} \{\hat{\phi}(x, 0) - I(x)\} - \hat{\lambda}(x, 0) = 0, \quad (16a)$$

$$W_{bc} \{\hat{\phi}(0, t) - B(t)\} - u \hat{\lambda}(0, t) = 0, \quad (16b)$$

$$W_{ob} \sum_{i=1}^M \{\hat{\phi}(x_i, t_i) - y_i\} \delta(x - x_i) \delta(t - t_i) - \left(\frac{\partial \hat{\lambda}}{\partial t} + u \frac{\partial \hat{\lambda}}{\partial x} \right) = 0, \quad (17)$$

$$\hat{\lambda}(x, T) = 0, \quad (17a)$$

$$\hat{\lambda}(L, t) = 0. \quad (17b)$$

(16) is the forward equation, (16a, 16b) are its initial/boundary conditions. (17) is the backward equation, (17a, 17b) are its conditions.

II: The weak constraint formulation

Construct a functional $J[\phi]$:

$$J[\phi] = W_{ic} \int_{x=0}^L dx \{\phi(x,0) - I(x)\}^2 + W_{bc} \int_{t=0}^T dt \{\phi(0,t) - B(t)\}^2 + \\ W_{ob} \sum_{i=1}^M \{\phi(x_i, t_i) - y_i\}^2 + W_e \int_{x=0}^L dx \int_{t=0}^T dt \left\{ \frac{\partial \phi}{\partial t} + u \frac{\partial \phi}{\partial x} - F \right\}^2. \quad (18)$$

What $\phi(x, t)$ makes $J[\phi]$ stationary?

Construct variations of J about the reference field $\hat{\phi}$, i.e.

$$J[\hat{\phi} + \delta\phi] = J[\hat{\phi}] + \delta J|_{\hat{\phi}}, \quad (19)$$

$$\delta J|_{\hat{\phi}} = \int_{x=0}^L dx \int_{t=0}^T dt \left. \frac{\partial J}{\partial \phi} \right|_{\hat{\phi}} \delta\phi + O(\delta\phi^2), \\ = 2W_{ic} \int_{x=0}^L dx \{\hat{\phi}(x,0) - I(x)\} \delta\phi(x,0) + \\ 2W_{bc} \int_{t=0}^T dt \{\hat{\phi}(0,t) - B(t)\} \delta\phi(0,t) + \\ 2W_{ob} \int_{x=0}^L dx \int_{t=0}^T dt \sum_{i=1}^M \{\hat{\phi}(x_i, t_i) - y_i\} \delta\phi(x, t) \delta(x - x_i) \delta(t - t_i) + \\ 2W_e \int_{x=0}^L dx \int_{t=0}^T dt \left\{ \frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} - F \right\} \left\{ \frac{\partial \delta\phi}{\partial t} + u \frac{\partial \delta\phi}{\partial x} \right\} + \quad (*) \\ O(\delta\phi^2). \quad (20)$$

Define:

$$\hat{\mu}(x, t) = W_e \left(\frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} - F \right), \quad (21)$$

where $\hat{\mu}(x, T) = 0$, $\hat{\mu}(L, t) = 0$. (*) of (20) is like (*) of (10) - rewrite using the integration by parts formula (11). (20) can becomes:

$$\delta J|_{\hat{\phi}} = 2W_{ic} \int_{x=0}^L dx \{\hat{\phi}(x,0) - I(x)\} \delta\phi(x,0) + 2W_{bc} \int_{t=0}^T dt \{\hat{\phi}(0,t) - B(t)\} \delta\phi(0,t) + \\ 2W_{ob} \int_{x=0}^L dx \int_{t=0}^T dt \sum_{i=1}^M \{\hat{\phi}(x_i, t_i) - y_i\} \delta\phi(x, t) \delta(x - x_i) \delta(t - t_i) - \\ 2 \int_{x=0}^L dx \hat{\mu}(x,0) \delta\phi(x,0) - 2 \int_{x=0}^L dx \int_{t=0}^T dt \frac{\partial \hat{\mu}}{\partial t} \delta\phi(x, t) - \\ 2 \int_{t=0}^T dt u \hat{\mu}(0, t) \delta\phi(0, t) - 2 \int_{t=0}^T dt \int_{x=0}^L dx u \frac{\partial \hat{\mu}}{\partial x} \delta\phi(x, t) + O(\delta\phi^2). \quad (22)$$

Setting the linear part of (22) to zero, using the model equation (1), and definition (21) gives Euler-Lagrange equations for the weak constraint:

$$\frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} - F = W_e^{-1} \hat{\mu}, \quad (23)$$

$$W_{ic} \{ \hat{\phi}(x, 0) - I(x) \} - \hat{\mu}(x, 0) = 0, \quad (23a)$$

$$W_{bc} \{ \hat{\phi}(0, t) - B(t) \} - u \hat{\mu}(0, t) = 0, \quad (23b)$$

$$W_{ob} \sum_{i=1}^M \{ \hat{\phi}(x_i, t_i) - y_i \} \delta(x - x_i) \delta(t - t_i) - \left(\frac{\partial \hat{\mu}}{\partial t} + u \frac{\partial \hat{\mu}}{\partial x} \right) = 0, \quad (24)$$

$$\hat{\mu}(x, T) = 0, \quad (24a)$$

$$\hat{\mu}(L, t) = 0. \quad (24b)$$

(23) is the forward equation, (13a, 23b) are its initial/boundary conditions. (24) is the backward equation, (24a, 24b) are its conditions.

Note: the strong constraint is a limit of the weak constraint in the limit when $W_e^{-1} \rightarrow 0$ (c.f. (23, 23a, 23b, 24, 24a, 24b) with (16, 16a, 16b, 17, 17a, 17b)).

Solving the Euler-Lagrange equations (23-24b) using the method of representers

Note: The forward equation (23) is solved for $\hat{\phi}(x, t)$ 'upwards and to the right' (Fig. 1); the backward equation (24) is solved for $\hat{\mu}(x, t)$ 'downwards and to the left' (Fig. 1).

Problem: In order to solve (23) $\hat{\mu}(x, t)$ is needed; in order to solve (24), $\hat{\phi}(x, t)$ is needed!

Define:

$$\left. \begin{array}{l} \text{Representer function } r_i(x, t) \\ \text{Backward representer function } \alpha_i(x, t) \end{array} \right\} \quad 1 \leq i \leq M,$$

(one representer and backward function per observation).

1. Solve the a-priori forward problem (2, 3, 4).

2. Solve the following simplified backward equations for the M backward representers $\alpha_i(x, t)$ 'downwards and to the left' (with impulses at the observation positions/times):

$$\delta(x - x_i) \delta(t - t_i) - \left(\frac{\partial \alpha_i}{\partial t} + u \frac{\partial \alpha_i}{\partial x} \right) = 0, \quad (25)$$

$$\alpha_i(x, T) = 0, \quad \alpha_i(L, t) = 0. \quad (25a, 25b)$$

3. Solve the following simplified forward equations for the M representers $r_i(x, t)$ 'upwards and to the right' (with $I(x) = 0, B(t) = 0, F = 0$):

$$\frac{\partial r_i}{\partial t} + u \frac{\partial r_i}{\partial x} = W_e^{-1} \alpha_i, \quad (26)$$

$$r_i(x, 0) = W_{ic}^{-1} \alpha_i(x, 0), \quad r_i(0, t) = W_{bc}^{-1} u \alpha_i(0, t). \quad (27a, 27b)$$

4. Look for a solution:

$$\hat{\phi}(x, t) = \phi_B(x, t) + \sum_{i=1}^M \beta_i r_i(x, t). \quad (28)$$

5. Act with $\partial / \partial t + u \partial / \partial x$ on (28), then use (23, 2, 26):

$$\begin{aligned} \frac{\partial \hat{\phi}}{\partial t} + u \frac{\partial \hat{\phi}}{\partial x} &= \frac{\partial \phi_B}{\partial t} + u \frac{\partial \phi_B}{\partial x} + \sum_{i=1}^M \beta_i \left(\frac{\partial r_i}{\partial t} + u \frac{\partial r_i}{\partial x} \right), \\ F + W_e^{-1} \hat{\mu} &= F + \sum_{i=1}^M \beta_i W_e^{-1} \alpha_i, \\ \hat{\mu}(x, t) &= \sum_{i=1}^M \beta_i \alpha_i(x, t). \end{aligned} \quad (29)$$

6. Substitute (29) into (24), then use (28, 25):

$$\begin{aligned} W_{\text{ob}} \sum_{i=1}^M \left\{ \hat{\phi}(x_i, t_i) - y_i \right\} \delta(x - x_i) \delta(t - t_i) &= \sum_{i=1}^M \beta_i \left(\frac{\partial \alpha_i}{\partial t} + u \frac{\partial \alpha_i}{\partial x} \right), \\ W_{\text{ob}} \sum_{i=1}^M \left\{ \phi_B(x_i, t_i) + \sum_{j=1}^M \beta_j r_j(x_i, t_i) - y_i \right\} \delta(x - x_i) \delta(t - t_i) &= \sum_{i=1}^M \beta_i \delta(x - x_i) \delta(t - t_i). \end{aligned} \quad (30)$$

7. Equate coefficients of impulses in (30):

$$\begin{aligned} W_{\text{ob}} \left\{ \phi_B(x_i, t_i) + \sum_{j=1}^M \beta_j r_j(x_i, t_i) - y_i \right\} &= \beta_i, \\ W_{\text{ob}} (\phi_B(x_i, t_i) - y_i) + \sum_{j=1}^M (W_{\text{ob}} r_j(x_i, t_i) - \delta_{ij}) \beta_j &= 0. \end{aligned} \quad (31)$$

8. Generate a matrix equation to solve for β_i (then used to generate solution via (28)):

$$\mathbf{W}_{\text{ob}} (\vec{\phi}_B^{\text{ob}} - \vec{y}) + (\mathbf{W}_{\text{ob}} \mathbf{P} - \mathbf{I}_M) \vec{\beta} = 0, \quad (32)$$

$$\text{where} \quad \mathbf{W}_{\text{ob}} = W_{\text{ob}} \mathbf{I}_M, \quad \vec{\phi}_B^{\text{ob}} = \begin{pmatrix} \phi_B(x_1, t_1) \\ \phi_B(x_2, t_2) \\ \dots \\ \phi_B(x_M, t_M) \end{pmatrix}, \quad \vec{y} = \begin{pmatrix} y_1 \\ y_2 \\ \dots \\ y_M \end{pmatrix}, \quad \vec{\beta} = \begin{pmatrix} \beta_1 \\ \beta_2 \\ \dots \\ \beta_M \end{pmatrix},$$

$$\mathbf{P} = \begin{pmatrix} r_1(x_1, y_1) & r_2(x_1, y_1) & \dots & r_M(x_1, y_1) \\ r_1(x_2, y_2) & r_2(x_2, y_2) & \dots & r_M(x_2, y_2) \\ \dots & \dots & \dots & \dots \\ r_1(x_M, y_M) & r_2(x_M, y_M) & \dots & r_M(x_M, y_M) \end{pmatrix}.$$