

## Differentiation of the cost-functional

The complete form of this minimization problem can be written as

$$\begin{aligned} \min_{p_1, p_2, \dots, p_M} J(p_1, p_2, \dots, p_M) = \\ \min_{p_1, p_2, \dots, p_M} \left( \frac{1}{2} \int_0^{t^*} \int_{\partial\Omega} [d(x, t) - v(x, t; p_1, p_2, \dots, p_M)]^2 dx dt \right) \end{aligned} \quad (1)$$

subject to the constraint that  $v$  solves

$$v_t + g_\alpha(\phi)I(v) = \nabla \cdot [k_\alpha(\phi)\nabla v] \quad \text{in } \Omega \quad (2)$$

$$k_\alpha(\phi)\nabla v \cdot n = 0 \quad \text{along } \partial\Omega \quad (3)$$

$$v(x, 0) = v_0(x) \quad \text{in } \Omega \quad (4)$$

where

$$\phi = \phi(x; p_1, p_2, \dots, p_M) = \sum_{i=1}^M p_i N_i(x), \quad (5)$$

$$g_\alpha(\phi) = H_\alpha(\phi) \approx \begin{cases} 0 & \text{if } x \text{ in } D \\ 1 & \text{if } x \text{ in } \Omega \setminus D \end{cases} \quad (6)$$

and

$$k_\alpha(\phi) = k_1(1 - H_\alpha(\phi)) + k_2 H_\alpha(\phi) \approx \begin{cases} k_1 & \text{if } x \text{ in } D \\ k_2 & \text{if } x \text{ in } \Omega \setminus D. \end{cases} \quad (7)$$

To obtain  $\frac{\partial J}{\partial p_i}$  we must differentiate the cost-functional with respect to  $p_i$ . Let  $i \in \{1, 2, \dots, M\}$  be arbitrary and define  $p = p_i$ . Now we see that

$$\frac{\partial J}{\partial p} = - \int_0^{t^*} \int_{\partial\Omega} [d(x, t) - v(x, t; p_1, \dots, p_M)] v_p(x, t; p_1, \dots, p_M) dx dt. \quad (8)$$

Next, let us look at the weak form of the problem (2)-(3): Find  $v$  such that

$$\int_0^{t^*} \int_{\Omega} v_t \psi dx dt + \int_0^{t^*} \int_{\Omega} g_\alpha(\phi) I(v) \psi dx dt + \int_0^{t^*} \int_{\Omega} k_\alpha(\phi) \nabla v \cdot \nabla \psi dx dt = 0, \quad (9)$$

for all test functions  $\psi \in V(\Omega)$ .

Now we differentiate (9) with respect to  $p$  and find that

$$\begin{aligned} & \int_0^{t^*} \int_{\Omega} v_{pt} \psi \, dx \, dt + \int_0^{t^*} \int_{\Omega} g'_\alpha(\phi) \phi_p I(v) \psi \, dx \, dt + \int_0^{t^*} \int_{\Omega} g_\alpha(\phi) I'(v) v_p \psi \, dx \, dt \\ & + \int_0^{t^*} \int_{\Omega} k'_\alpha(\phi) \phi_p \nabla v \cdot \nabla \psi \, dx \, dt + \int_0^{t^*} \int_{\Omega} k_\alpha(\phi) \nabla v_p \cdot \nabla \psi \, dx \, dt = 0, \end{aligned} \quad (10)$$

for all  $\psi \in V(\Omega)$ , and we use (6)-(7) to get

$$\begin{aligned} & \int_0^{t^*} \int_{\Omega} v_{pt} \psi \, dx \, dt + \int_0^{t^*} \int_{\Omega} g_\alpha(\phi) I'(v) v_p \psi \, dx \, dt + \int_0^{t^*} \int_{\Omega} k_\alpha(\phi) \nabla v_p \cdot \nabla \psi \, dx \, dt \\ & = - \int_0^{t^*} \int_{\Omega} \delta_\alpha(\phi) \phi_p I(v) \psi \, dx \, dt - \int_0^{t^*} \int_{\Omega} (k_2 - k_1) \delta_\alpha(\phi) \phi_p \nabla v \cdot \nabla \psi \, dx \, dt. \end{aligned} \quad (11)$$

Introducing the operator

$$a(\xi, \psi) = \int_0^{t^*} \int_{\Omega} \xi_t \psi \, dx \, dt + \int_0^{t^*} \int_{\Omega} g_\alpha(\phi) I'(v) \xi \psi \, dx \, dt + \int_0^{t^*} \int_{\Omega} k_\alpha(\phi) \nabla \xi \cdot \nabla \psi \, dx \, dt$$

for  $\xi, \psi \in V(\Omega)$ , equation (11) may be written on the form

$$a(v_p, \psi) = - \int_0^{t^*} \int_{\Omega} \left( I(v) \psi + (k_2 - k_1) \nabla v \cdot \nabla \psi \right) \delta_\alpha(\phi) \phi_p \, dx \, dt. \quad (12)$$

Next, let  $w$  denote the solution of the following auxiliary problem; find  $w \in V(\Omega)$  such that

$$a(\psi, w) = - \int_0^{t^*} \int_{\partial\Omega} [d(x, t) - v(x, t; p_1, \dots, p_M)] \psi(x, t) \, dx \, dt. \quad (13)$$

By choosing  $\psi = v_p$  in (13) we find from (8) that

$$\frac{\partial J}{\partial p} = a(v_p, w). \quad (14)$$

Further (12) and (14) imply that

$$\frac{\partial J}{\partial p} = - \int_0^{t^*} \int_{\Omega} \left( I(v) w + (k_2 - k_1) \nabla v \cdot \nabla w \right) \delta_\alpha(\phi) \phi_p \, dx \, dt. \quad (15)$$

We thus conclude that the partial derivatives  $\partial J / \partial p_1, \partial J / \partial p_2, \dots, \partial J / \partial p_M$  of  $J$  can be computed by the following procedure;

- a) Solve (9) for  $v$
- b) Solve (13) for  $w$
- c) For  $i = 1, 2, \dots, M$ , compute

$$\frac{\partial J}{\partial p_i} = - \int_0^{t^*} \int_{\Omega} \left( I(v)w + (k_2 - k_1)\nabla v \cdot \nabla w \right) \delta_\alpha(\phi) \phi_{p_i} dx dt. \quad (16)$$

The complexity of this method is (almost) independent of the number  $M$  of infarction parameters!

Note that the classical form of the adjoint problem (13) reads

$$-w_t + g_\alpha(\phi)I'(v)w = \nabla \cdot [k_\alpha \nabla w] \quad \text{in } \Omega \quad (17)$$

$$k_\alpha(\phi) \nabla w \cdot n = -(d - v) \quad \text{along } \partial\Omega \quad (18)$$

$$w(x, t^*) = 0 \quad \text{in } \Omega. \quad (19)$$

We find the classical form of the adjoint problem

$$a(\psi, w) = - \int_0^{t^*} \int_{\partial\Omega} [d(x, t) - v(x, t; p_1, \dots, p_M)] \psi dx dt, \quad \text{for all } \psi \in V(\Omega)$$

by using the operator

$$a(\psi, w) = \int_0^{t^*} \int_{\Omega} \psi_t w dx dt + \int_0^{t^*} \int_{\Omega} g_\alpha(\phi)I'(v)\psi w dx dt + \int_0^{t^*} \int_{\Omega} k_\alpha(\phi) \nabla \psi \cdot \nabla w dx dt.$$

Now, integrating by parts (the first term) and using Green's lemma (the third term) we get

$$\begin{aligned} & \left[ \int_{\Omega} \psi w dx \right]_{t=0}^{t=t^*} - \int_0^{t^*} \int_{\Omega} \psi w_t dx dt + \int_0^{t^*} \int_{\Omega} g_\alpha(\phi)I'(v)\psi w dx dt \\ & + \int_0^{t^*} \int_{\partial\Omega} k_\alpha(\phi) \psi \nabla w \cdot n dx dt + \int_0^{t^*} \int_{\Omega} \nabla \cdot [k_\alpha(\phi) \nabla w] \psi dx dt = - \int_0^{t^*} \int_{\partial\Omega} [d - v] \psi dx dt. \end{aligned}$$

By choosing appropriate test functions  $\psi$ , we will end up with the classical form (17)-(19).