1 Advection-Diffusion constrained optimization problems

Let us consider the problem:

$$\begin{aligned}
\min_{\rho,\vec{w}} \quad & \frac{1}{2}\int_0^T \int_\Omega (\rho-\hat{\rho})^2\,dxdt + \frac{\beta}{2}\int_0^T\int_\Omega \|\vec{w}\|^2\,dxdt \\
\text{s.t} \quad & \partial_t\rho - \nabla^2\rho = -\nabla\cdot(\rho\vec{w}) + \nabla\cdot(\rho\nabla V_{ext}), \\
& \rho = \rho_0 \quad \text{at } t=0, \\
& \rho = 0 \quad \text{on } \partial\Omega. \qquad (1)
\end{aligned}$$

The state and target variables are denoted ρ and $\hat{\rho}$ respectively. Our control is the vector $\vec{w} = [w_1, w_2]$ for 2D problems and $\vec{w} = [w_1, w_2, w_3]$ for 3D problems, and β is the regularization parameter. We obtain the optimality system by introducing two Lagrange multipliers p_1 and p_2 corresponding to the interior and boundary of Ω, respectively, and consider the Lagrangian

$$\begin{aligned}
\mathcal{L}(\rho,\vec{w},p_1,p_2) = & \frac{1}{2}\int_0^T \int_\Omega (\rho-\hat{\rho})^2\,dxdt + \frac{\beta}{2}\int_0^T\int_\Omega \|\vec{w}\|^2\,dxdt \\
& - \int_0^T\int_\Omega \big(\partial_t\rho - \nabla^2\rho + \nabla\cdot(\rho\vec{w}) - \nabla\cdot(\rho\nabla V_{ext})\big)\,p_1\,dxdt \\
& - \int_0^T\int_{\partial\Omega} \rho p_2\,dsdt. \qquad (2)
\end{aligned}$$

We find the Fréchet derivative with respect to ρ and $\vec{w}$ in the direction h:

$$\begin{aligned}
D_\rho\mathcal{L}(\rho,\vec{w},p_1,p_2)h = & \int_0^T\int_\Omega (\rho-\hat{\rho})h\,dxdt \\
& - \int_0^T\int_\Omega \big(\partial_t h - \nabla^2 h + \nabla\cdot(h\vec{w}) - \nabla\cdot(h\nabla V_{ext})\big)\,p_1\,dxdt \\
& - \int_0^T\int_{\partial\Omega} hp_2\,dsdt \\
= & \int_0^T\int_\Omega (\rho-\hat{\rho})h\,dxdt \\
& + \int_0^T\int_\Omega \big(h\partial_t p_1 + h\nabla^2 p_1 + h\vec{w}\cdot\nabla p_1 - h\nabla V_{ext}\cdot\nabla p_1\big)\,dxdt \\
& + \int_0^T\int_{\partial\Omega} \left(p_1\frac{\partial h}{\partial n} - h\frac{\partial p_1}{\partial n} - hp_1\vec{w}\cdot\vec{n} + hp_1\frac{\partial V_{ext}}{\partial n}\right)dsdt \\
& - \int_0^T\int_{\partial\Omega} p_2 h\,dsdt.
\end{aligned}$$

and for w_i, $i = 1, 2, \dots$:

$$\begin{aligned} D_{w_i}\mathcal{L}(\rho, w_i, p_1, p_2)h &= \int_0^T \int_\Omega -\beta w_i + \frac{\partial}{\partial x_i}(\rho h) p_1 \, dxdt \\ &= \int_0^T \int_\Omega -\beta w_i + \frac{\partial}{\partial x_i}(\rho h p_1) - \rho h \frac{\partial p_1}{\partial x_i} \, dxdt. \end{aligned}$$

For a stationary point, the optimal state and control $\bar{\rho}$ and $\bar{\vec{w}}$ must satisfy

$$D_\rho \mathcal{L}(\bar{\rho}, \bar{\vec{w}}, p_1, p_2)h = 0 \quad \forall h \in \mathcal{H}^1(\Omega) \tag{3}$$

and

$$D_{\vec{w}} \mathcal{L}(\bar{\rho}, \bar{\vec{w}}, p_1, p_2)h = 0 \quad \forall h \in L^2(\Omega). \tag{4}$$

In particular, for all $h \in C_0^\infty(\Omega)$, $h|_{\partial\Omega} = 0 = \frac{\partial h}{\partial n}|_{\partial\Omega}$. So, (3) and (4) reduce to

$$\begin{aligned} -\partial_t p_1 - \nabla^2 p_1 - \vec{w} \cdot \nabla p_1 + \nabla V_{ext} \cdot \nabla p_1 = \rho - \hat{\rho} \quad \text{and} \\ \beta \vec{w} - \rho \nabla p_1 = 0. \end{aligned}$$

If we label p_1 as p then we can write the adjoint equation as

$$\begin{aligned} -\partial_t p - \nabla^2 p - \vec{w} \cdot \nabla p + \nabla V_{ext} \cdot \nabla p = \rho - \hat{\rho}, \\ p = 0 \quad \text{at } t = T, \\ p = 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{5}$$

and almost everywhere:

$$\beta \vec{w} + \rho \nabla p = 0.$$

The optimality system for problem (1) becomes the *state equation*:

$$\begin{aligned} \partial_t \rho - \nabla^2 \rho = -\nabla \cdot (\rho \vec{w}) + \nabla \cdot (\rho \nabla V_{ext}), \\ \rho = \rho_0 \quad \text{at } t = 0, \\ \rho = 0 \quad \text{on } \partial\Omega, \end{aligned}$$

the *adjoint equation*:

$$\begin{aligned} -\partial_t p - \nabla^2 p = \vec{w} \cdot \nabla p - \nabla V_{ext} \cdot \nabla p + \rho - \hat{\rho}, \\ p = 0 \quad \text{at } t = T, \\ p = 0 \quad \text{on } \partial\Omega, \end{aligned}$$

and the *gradient equation*:

$$\beta \vec{w} + \rho \cdot \nabla p = 0.$$

1.1 With a nonlocal (integral) term

We now introduce a nonlocal term (in terms of ρ) into the problem

$$\begin{aligned} \min_{\rho,\vec{w}} \quad & \frac{1}{2}\int_0^T \int_\Omega (\rho - \hat{\rho})^2 \, dxdt + \frac{\beta}{2}\int_0^T \int_\Omega \|\vec{w}\|^2 \, dxdt \\ \text{s.t} \quad & \partial_t \rho - \nabla^2 \rho + \nabla \cdot (\rho \vec{w}) - \nabla \cdot (\rho \nabla V_{ext}) - \nabla \cdot \left(\int_\Omega \rho(r)\rho(s)\vec{K}(|r-s|)ds \right) = 0, \\ & \rho = \rho_0 \quad \text{at } t = 0, \\ & \rho = 0 \quad \text{on } \partial\Omega, \end{aligned} \tag{6}$$

where $\vec{K}$ denotes a vector function. The other terms turn out the same in the adjoint and gradient equations so we focus here on the nonlocal term. If we let p be the first Lagrange multiplier then the term we are interested in is

$$\mathcal{L}(\rho, \vec{w}, p, p_2) = \cdots - \int_{[0,T]\times\Omega} p(r)\nabla_r \cdot \left(\int_\Omega \rho(r)\rho(s)\vec{K}(|r-s|)ds \right) dr + \cdots$$

The Fréchet derivative of the product $\rho(r)\rho(s)$ in the direction h is

$$\lim_{\epsilon \to 0} \frac{(\rho(r) + \epsilon h(r))(\rho(s) + \epsilon h(s)) - \rho(r)\rho(s)}{\epsilon} = \rho(r)h(s) + \rho(s)h(r).$$

Hence the Fréchet derivative of the Lagrangian in terms ρ in the direction h becomes

$$D_\rho \mathcal{L}(\rho, \vec{w}, p, p_2) = \cdots - \int_{[0,T]\times\Omega} p(r)\nabla_r \cdot \left(\int_{[0,T]\times\Omega} (\rho(r)h(s) + h(r)\rho(s))\vec{K}(|r-s|)ds \right) dr + \cdots$$

Using the identity

$$\nabla \cdot (a\vec{b}) = a\nabla \cdot \vec{b} + \nabla a \cdot \vec{b}$$

along with the argument that $\nabla_r \cdot \left(p(r) \left(\int_{[0,T]\times\Omega} (\rho(r)h(s) + h(r)\rho(s))\vec{K}(|r-s|)ds \right) \right)$ becomes boundary terms and eventually zero due to integration by parts, the Divergence theorem, and the boundary condition $p = 0$, we are left with

$$
\begin{aligned}
D_\rho \mathcal{L}(\rho, \vec{w}, p, p_2) &= \cdots + \int_{[0,T]\times\Omega} \left(\int_{[0,T]\times\Omega} (\rho(r)h(s) + h(r)\rho(s)) \vec{K}(|r-s|) ds \right) \cdot \nabla_r p(r) dr + \cdots \\
&= \cdots + \int_{[0,T]\times\Omega} h(r) \left(\int_{[0,T]\times\Omega} \rho(s) \vec{K}(|r-s|) ds \right) \cdot \nabla_r p(r) dr \\
&\quad + \int_{[0,T]\times\Omega} h(s) \left(\int_{[0,T]\times\Omega} \rho(r) \vec{K}(|r-s|) \cdot \nabla_r p(r) dr \right) ds + \cdots \\
&= \cdots + \int_{[0,T]\times\Omega} h(r) \left(\int_{[0,T]\times\Omega} \rho(s) \vec{K}(|r-s|) ds \right) \cdot \nabla_r p(r) dr \\
&\quad + \int_{[0,T]\times\Omega} h(r) \left(\int_{[0,T]\times\Omega} \rho(s) \vec{K}(|r-s|) \cdot \nabla_s p(s) ds \right) dr + \cdots
\end{aligned}
$$

Hence the optimality system of problem (6) is the state equation:

$$
\begin{aligned}
&\partial_t \rho - \nabla^2 \rho + \nabla \cdot (\rho \vec{w}) - \nabla \cdot (\rho \nabla V_{ext}) - \nabla \cdot \left(\int_{[0,T]\times\Omega} \rho(r)\rho(s) \vec{K}(|r-s|) ds \right) = 0, \\
&\rho = \rho_0 \quad \text{at } t = 0, \\
&\rho = 0 \quad \text{on } \partial\Omega,
\end{aligned} \tag{7}
$$

the adjoint equation:

$$
\begin{aligned}
&\partial_t p + \nabla^2 p + \vec{w} \cdot \nabla p - \nabla V_{ext} \cdot \nabla p - \left(\int_{[0,T]\times\Omega} \rho(s) \vec{K}(|r-s|) ds \right) \cdot \nabla_r p(r) \\
&\quad - \int_{[0,T]\times\Omega} \Big(\rho(s) \vec{K}(|r-s|) \cdot \nabla_s p(s) \Big) ds - \rho + \hat{\rho} = 0, \\
&p = 0 \quad \text{at } t = T, \\
&p = 0 \quad \text{on } \partial\Omega,
\end{aligned} \tag{8}
$$

and the gradient equation:

$$
\beta \vec{w} + \rho \cdot \nabla p = 0. \tag{9}
$$