Deriving Optimality Conditions that slightly differ from the usual ones

We consider time independent flow control, control through the external potential and a target that is only considered at the final time rather than over the whole time horizon.

1 Time independent flow control

We have the following OCP:

$$
\begin{aligned}
&J = \frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_\Omega \mathbf{w}(r)^2 dr \\
&\text{subject to:} \\
&\frac{\partial \rho}{\partial t} = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w}(r))
\end{aligned}
$$

Then the Lagrangian is:

$$
\begin{aligned}
\mathcal{L}(\rho, \mathbf{w}, q) = &\frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_\Omega \mathbf{w}(r)^2 dr \\
&- \int_0^T \int_\Omega q\frac{\partial \rho}{\partial t} - q\nabla^2\rho + q\nabla \cdot (\rho \mathbf{w}) dr dt.
\end{aligned}
$$

And after integrating by parts (neglecting the BCs because they are unchanged from before):

$$
\begin{aligned}
\mathcal{L}(\rho, \mathbf{w}, q) = &\frac{1}{2}\int_0^T \int_\Omega (\rho - \widehat{\rho})^2 dr dt + \frac{\beta}{2}\int_\Omega \mathbf{w}(r)^2 dr \\
&- \int_0^T \int_\Omega q\frac{\partial \rho}{\partial t} - q\nabla^2\rho - \rho \mathbf{w} \cdot \nabla q dr dt.
\end{aligned}
$$

Taking derivatives with respect to $\mathbf{w}$ gives:

$$
\mathcal{L}_{\mathbf{w}}(\rho, \mathbf{w}, q)h = \int_\Omega \beta \mathbf{w}(r)\cdot \mathbf{h}(r) dt + \int_0^T \int_\Omega \rho \mathbf{h}(r) \cdot \nabla q dr dt.
$$

Since $\mathbf{w}$ does not depend on t, neither does $\mathbf{h}$ and so this can be taken out of the time integral:

$$
\mathcal{L}_{\mathbf{w}}(\rho, \mathbf{w}, q)h = \int_\Omega \left(\beta \mathbf{w}(r)\cdot \mathbf{h}(r) + \mathbf{h}(r) \cdot \int_0^T \rho \nabla q dt\right) dr.
$$

Then we get:

$$
\beta \mathbf{w}(r) + \int_0^T \rho \nabla q dt = 0
$$

And finally:

$$
\mathbf{w}(r) = -\frac{1}{\beta}\int_0^T \rho \nabla q dt
$$

2 V_{ext} control

We have the following OCP:

$$J = \frac{1}{2}\int_0^T\int_\Omega (\rho - \widehat{\rho})^2 drdt + \frac{\beta}{2}\int_0^T\int_\Omega V_{ext}^2 dr$$

subject to:

$$\frac{\partial \rho}{\partial t} = \nabla^2\rho + \nabla\cdot(\rho\nabla V_{ext})$$

The Lagrangian is:

$$\begin{aligned}\mathcal{L}(\rho, V_{ext}, q) &= \frac{1}{2}\int_0^T\int_\Omega (\rho - \widehat{\rho})^2 drdt + \frac{\beta}{2}\int_0^T\int_\Omega V_{ext}^2 dr \\ &- \int_0^T\int_\Omega q\frac{\partial \rho}{\partial t} - q\nabla^2\rho - q\nabla\cdot(\rho\nabla V_{ext})drdt.\end{aligned}$$

We need to integrate by parts twice to get the term in V_{ext} into the necessary form:

$$\begin{aligned}\int_0^T\int_\Omega q\nabla\cdot(\rho\nabla V_{ext})drdt &= \int_0^T\int_{\partial\Omega} q\rho\nabla V_{ext}\cdot\mathbf{n}drdt - \int_0^T\int_\Omega \rho\nabla V_{ext}\cdot\nabla q drdt \\ &= \int_0^T\int_{\partial\Omega} q\rho\nabla V_{ext}\cdot\mathbf{n} - \rho V_{ext}\nabla q\cdot\mathbf{n}drdt + \int_0^T\int_\Omega V_{ext}\nabla\cdot(\rho\nabla q)drdt\end{aligned}$$

We will also have

$$\int_0^T\int_\Omega q\nabla^2\rho = \int_0^T\int_{\partial\Omega} q\nabla\rho\cdot\mathbf{n} - \rho\nabla q\cdot\mathbf{n}drdt + \int_0^T\int_\Omega \rho\nabla^2 q drdt$$

2.1 Boundary Conditions

And the boundary conditions:

$$\int_0^T\int_{\partial\Omega} q_{\partial\Omega}\nabla\rho\cdot\mathbf{n} + q_{\partial\Omega}\rho\nabla V_{ext}\cdot\mathbf{n}drdt$$

Combining these:

$$\int_0^T\int_{\partial\Omega} q\rho\nabla V_{ext}\cdot\mathbf{n} - \rho V_{ext}\nabla q\cdot\mathbf{n} + q\nabla\rho\cdot\mathbf{n} - \rho\nabla q\cdot\mathbf{n} + q_{\partial\Omega}\nabla\rho\cdot\mathbf{n} + q_{\partial\Omega}\rho\nabla V_{ext}\cdot\mathbf{n}drdt$$

During the derivation of the adjoint equation we have:

$$\int_0^T\int_{\partial\Omega}\mathbf{n}\cdot h\Big(q\nabla V_{ext} - V_{ext}\nabla q - \nabla q + q_{\partial\Omega}\nabla V_{ext}\Big) + \nabla h\cdot\mathbf{n}\Big(q + q_{\partial\Omega}\Big)drdt$$

Then from the ∇h terms we get $q_{\partial\Omega} = -q$ and so:

$$(q\nabla V_{ext} - V_{ext}\nabla q - \nabla q - q\nabla V_{ext})\cdot\mathbf{n} = 0$$

And therefore the new adjoint boundary condition is:

$$(1 + V_{ext})\frac{\partial q}{\partial n} = 0.$$

2.2 Gradient Equation

We take the derivative of the Lagrangian with respect to V_{ext}:

$$\mathcal{L}_{V_{ext}}(\rho, V_{ext}, q)h = \int_0^T \int_\Omega \beta V_{ext} h + \nabla \cdot (\rho \nabla q) h dr dt$$

Then we have:

$$\beta V_{ext} + \nabla \cdot (\rho \nabla q) = 0$$

And finally

$$V_{ext} = -\frac{1}{\beta} \nabla \cdot (\rho \nabla q).$$

3 Target at final time

We consider the following OCP, where $\widehat{\rho}$ does not depend on time; we are only interested in the target at the final time T. The problem reads:

$$J = \frac{1}{2} \int_\Omega (\rho(T) - \widehat{\rho})^2 dr + \frac{\beta}{2} \int_0^T \int_\Omega \mathbf{w}^2 dr$$

subject to:

$$\frac{\partial \rho}{\partial t} = \nabla^2 \rho - \nabla \cdot (\rho \mathbf{w})$$

Then the Lagrangian is:

$$\begin{aligned} \mathcal{L}(\rho, \mathbf{w}, q) = &\frac{1}{2} \int_\Omega (\rho(T) - \widehat{\rho})^2 dr + \frac{\beta}{2} \int_0^T \int_\Omega \mathbf{w}^2 dr \\ &- \int_0^T \int_\Omega q \frac{\partial \rho}{\partial t} - q \nabla^2 \rho + q \nabla \cdot (\rho \mathbf{w}) dr dt. \end{aligned}$$

From integrating by parts we get:

$$\int_0^T \int_\Omega -q \frac{\partial \rho}{\partial t} dr dt = - \int_\Omega q(T)\rho(T) - q(0)\rho(0) dr + \int_0^T \int_\Omega \rho \frac{\partial q}{\partial t} dr dt$$

$$\begin{aligned} \mathcal{L}(\rho, \mathbf{w}, q) = &\frac{1}{2} \int_\Omega (\rho(T) - \widehat{\rho})^2 dr + \frac{\beta}{2} \int_0^T \int_\Omega \mathbf{w}^2 dr \\ &- \int_\Omega q(T)\rho(T) - q(0)\rho(0) dr + \int_0^T \int_\Omega \rho \frac{\partial q}{\partial t} + q \nabla^2 \rho - q \nabla \cdot (\rho \mathbf{w}) dr dt. \end{aligned}$$

Taking the derivative with respect to ρ gives:

$$\begin{aligned} \mathcal{L}_\rho(\rho, \mathbf{w}, q)h = &\int_\Omega (\rho(T) - \widehat{\rho}) h(T) dr - \int_\Omega q(T) h(T) dr \\ &+ \int_0^T \int_\Omega h \frac{\partial q}{\partial t} + q \nabla^2 h - q \nabla \cdot (h \mathbf{w}) dr dt. \end{aligned}$$

Considering the terms for $h(T)$, we get:

$$(\rho(T) - \widehat{\rho}) - q(T) = 0,$$

and so

$$q(T) = \rho(T) - \widehat{\rho}.$$

The adjoint PDE remains unchanged, except for the fact that $\rho - \widehat{\rho}$ does not enter the PDE anymore.