ADJOINT-BASED GRADIENT FOR TIME-DEPENDENT PROBLEMS

We consider an inverse problem governed by a time-dependent forward problem in the form of the time-dependent balance of energy equation:

$$\min_{m \in H^1} \Phi(m) := \frac{1}{2}\int_0^T\int_\Omega (Bu-d)^2 \, dx\, dt + \frac{\beta_T}{2}\int_\Omega \nabla m_T \cdot \nabla m_T \, dx + \frac{\beta_I}{2}\int_\Omega \nabla m_I \cdot \nabla m_I \, dx$$

where u depends on m through the solution of the energy equation

$$\rho c \frac{\partial u}{\partial t} + \rho c v \cdot \nabla u - \nabla \cdot (m_T \nabla u) = 0 \quad \text{in } \Omega \times (0,T] \quad \text{(PDE)}$$

$$u(x,t) = 0 \quad \text{on } \Gamma \times (0,T] \quad \text{(BC)}$$

$$u(x,0) = m_I \quad \text{in } \Omega \quad \text{(IC)}$$

Here, B is a space-time observation operator, i.e. it prescribes locations in space and instants in time at which observations are made

d is the data at these locations/instants

$m_T = m_T(x)$ is the thermal conductivity inversion parameter

$m_I = m_I(x)$ is the initial condition inversion parameter

ρ & c are the density and specific heat, respectively (known)

$u = u(x,t)$ is the temperature (state) variable

$v = v(x,t)$ is the (known) velocity field

So we are inverting for both the initial condition $m_I(x)$ (this is often called state estimation) and the thermal conductivity parameter $m_T(x)$ (often called parameter estimation).

We next proceed to form the Lagrangian, which involves Φ and the weak form of the forward energy equation. To obtain the weak form of the forward problem, we multiply by the Lagrange multiplier/adjoint variable $p(x,t)$ and integrate over the space-time domain:

$$\underbrace{\int_0^T\int_\Omega}_{\text{space-time}} \overset{p=p(x,t)}{p}\left[\rho c\frac{\partial u}{\partial t} + \rho c\, v\cdot\nabla u - \nabla\cdot(m_T\nabla u)\right]dx\,dt = 0 \quad \forall\, p(x,t)\in\mathcal{P}$$

where $\mathcal{P}$ is the space of admissible functions for $p(x,t)$, namely $H^1(\Omega)\times L^2(0,T)$. We integrate the diffusion term in space to balance the derivatives on u and p:

$$\int_0^T\int_\Omega\left[p\rho c\frac{\partial u}{\partial t} + p\rho c\, v\cdot\nabla u + m_T\nabla u\cdot\nabla p\right]dx\,dt - \int_0^T\int_\Gamma p\, m_T\nabla u\cdot n\, ds\,dt = 0 \quad \forall p\in\mathcal{P}$$

Notice that we do not take $p=0$ on Γ; even though this will be the case (since the observations are in the interior), we want to allow this condition to emerge. So p is arbitrary on Γ (for all time). Notice also that this is different from the usual weak form in finite elements, where the "test function" p is a function of space only. Here, $p(x,t)$ represents the Lagrange multiplier, and so it is defined everywhere where the residual is defined, i.e. $\Omega\times(0,T]$.

The Lagrangian is thus defined as:

$$\boxed{\begin{aligned}\mathcal{L}(u,p,m_T,m_I,q) := {}& \frac{1}{2}\int_0^T\int_\Omega (Bu-d)^2\,dx\,dt + \frac{\beta_T}{2}\int_\Omega \nabla m_T\cdot\nabla m_T\,dx \\ &+ \frac{\beta_I}{2}\int_\Omega \nabla m_I\cdot\nabla m_I\,dx + \int_0^T\int_\Omega\left[p\rho c\frac{\partial u}{\partial t} + p\rho c\, v\cdot\nabla u + m_T\nabla u\cdot\nabla p\right]dx\,dt \\ &- \int_0^T\int_\Gamma p\, m_T\nabla u\cdot n\, ds\,dt + \int_\Omega \overset{q=q(x),\ \text{Lagrange multiplier for I.C.}}{q}\underbrace{(u(x,0)-m_I)}_{\text{the residual of the IC}}\,dx,\end{aligned}}$$

where $u \in \mathcal{U} := H_0^1(\Omega) \times L^2(0,T)$, $p \in \mathcal{P}$, $m_T \in H^1(\Omega)$, $m_I \in H^1(\Omega)$, $q \in L^2(\Omega)$.

Notice the last term in the Lagrangian: it enforces the initial condition $u(x,0) = m_I(x)$ via the Lagrange multiplier $q(x)$, which is defined only as a spatial function since m_I is a function of space only. This is critical in order to "expose" $m_I(x)$ to the Lagrangian.

Now we take variations of the Lagrangian w.r.t. p, q, u, m_T, m_I:

$$\left.\begin{array}{ll} \delta_p \mathcal{L} = 0 & \forall \hat{p} \in \mathcal{U} \\ \delta_q \mathcal{L} = 0 & \forall \hat{q} \in L^2(\Omega) \end{array}\right\}$$

these just return the forward problem, which you can confirm by reverse integrating by parts

$\delta_u \mathcal{L} = 0 \quad \forall \hat{u} \in \mathcal{U} \Rightarrow$ Weak form of the adjoint equation: Find $u \in \mathcal{U}$ s.t.

$$\boxed{\begin{aligned} &\int_0^T\int_\Omega (Bu-d)B\hat{u}\,dx\,dt + \int_0^T\int_\Omega \left[p\rho c\frac{\partial \hat{u}}{\partial t} + p\rho c v\cdot\nabla\hat{u} + m_T\nabla\hat{u}\cdot\nabla p\right]dx\,dt \\ &- \int_0^T\int_\Gamma p\, m_T \nabla\hat{u}\cdot n\, ds\, dt + \int_\Omega q\,\hat{u}(x,0)\,dx = 0 \quad \forall \hat{u} \in \mathcal{U} \end{aligned}}$$

To derive the strong form, we begin by integrating by parts to isolate the $\hat{u}$:

$$\int_0^T\int_\Omega \hat{u}\left[B^*(Bu-d) - \rho c\frac{\partial p}{\partial t} - \rho c\nabla\cdot(pv) - \nabla\cdot(m_T\nabla p)\right]dx\,dt$$

$$+ \int_0^T\int_\Gamma \cancel{\hat{u}}\left[\rho c\, p v\cdot n + m_T\nabla p\cdot n\right]ds\,dt + \underbrace{\int_\Omega\left[\hat{u}(x,T)\rho c\, p(x,T) - \hat{u}(x,0)\rho c\, p(x,0)\right]dx}_{\text{from integrating } \frac{\partial}{\partial t} \text{ term by parts}}$$

0 (since $\hat{u} = 0$ on Γ)

$$- \int_0^T\int_\Gamma p\, m_T\nabla\hat{u}\cdot n\, ds\, dt + \int_\Omega q\,\hat{u}(x,0)\,dx = 0 \quad \forall \hat{u} \in \mathcal{U}$$

$$\Rightarrow \int_0^T \int_\Omega \overset{\hat u \text{ is arbitrary in } \Omega\times(0,T]}{\hat u}\; \overbrace{\left[B^*(Bu-d) - \rho c \frac{\partial p}{\partial t} - \rho c \nabla\cdot(p v) - \nabla\cdot(m_T \nabla p)\right]}^{\Rightarrow\, = 0 \text{ in } \Omega\times(0,T]} dx\,dt$$

$$+ \int_\Omega \overbrace{\hat u(x,T)}^{\text{arb. in } \Omega \text{ at } t=T} \underbrace{\rho c\, p(x,T)}_{\substack{\Rightarrow\, = 0 \text{ in } \Omega \\ \text{at } t=T}} dx + \int_\Omega \overbrace{\hat u(x,0)}^{\text{arb in } \Omega \text{ at } t=0} \underbrace{\left[q - \rho c\, p(x,0)\right]}_{\Rightarrow\, = 0 \text{ in } \Omega \text{ at } t=0} dx - \int_0^T \int_\Gamma \underbrace{p}_{\substack{\Rightarrow\, = 0 \\ \text{on } \Gamma\times(0,T]}} \overbrace{m_T \nabla \hat u \cdot n}^{\text{arb. on } \Gamma\times(0,T]}\, ds\,dt = 0 \quad \forall \hat u \in \mathcal{U}$$

Now we can state the strong form of the adjoint equation:

- $\hat u(x,t)$ is arbitrary in $\Omega\times(0,T]$:

$$-\rho c \frac{\partial p}{\partial t} - \rho c \nabla\cdot(p v) - \nabla\cdot(m_T \nabla p) = -B^*(Bu-d) \quad \text{in } \Omega\times(0,T] \qquad \text{PDE}$$

- $m_T \nabla \hat u \cdot n$ is arbitrary on $\Gamma\times(0,T]$:

$$p = 0 \qquad \text{on } \Gamma\times(0,T] \qquad \text{BC}$$

- $\hat u(x,T)$ is arbitrary in Ω at $t=T$ (and $\rho c \neq 0$):

$$p(x,T) = 0 \qquad \text{in } \Omega \text{ at } t=T \qquad \text{Terminal value}$$

Finally, we argue that $\hat u(x,0)$ is arbitrary in Ω at $t=0$, and thus

$$\boxed{q(x) = \rho c\, p(x,0) \quad \text{in } \Omega}$$

This gives the <u>definition of the Lagrange multiplier</u> for enforcing the initial condition, $q(x)$, in terms of the value of the adjoint at $t=0$.

Note that the adjoint equation can be seen to be a <u>terminal value problem</u> (as opposed to an initial value problem) since the value of p is specified not at $t=0$, but at $t=T$. This equation is thus solved backward in time. But don't worry, it is stable backward in time, because its operator is the adjoint of the forward operator —

note that time has been reversed ($-\partial/\partial t$), and the advection term has also been reversed ($-\nabla\cdot(v\,\cdot)$). So solving the adjoint energy equation backward in time is equivalent to solving the forward problem, forward in time (modulo source terms, and for a linear forward problem), as can be seen by defining a new time variable that is opposite in direction to t.

Finally, we take $\delta_{m_T}\mathcal{L} = 0$ and $\delta m_I \mathcal{L} = 0$ to derive the two components of the gradient:

$\delta_{m_T}\mathcal{L} = 0 \;\; \forall\, m_T \in H^1 \Rightarrow$ Weak form of gradient w.r.t. m_T:

$$\boxed{\left(\mathcal{G}_T(m), \hat{m}_T\right) := \beta_T \int_\Omega \nabla m_T \cdot \nabla \hat{m}_T \, dx + \int_0^T\!\!\int_\Omega \hat{m}_T \nabla u \cdot \nabla p \, dx\, dt \quad \forall\, \hat{m}_T \in H^1}$$

Note in the expression above, we did not include the term $-\int_0^T\!\!\int_\Gamma p \hat{m}_T \nabla u \cdot n \, ds\, dt$. This is because, in deriving the adjoint, we determined that $p = 0$ on $\Gamma \times (0,T]$. The strong form of the gradient can be derived by integrating the first term by parts to isolate $\hat{m}_T$, and arguing that $\hat{m}_T$ is arbitrary in Ω:

$$\left(\mathcal{G}_T(m), \hat{m}_T\right) := \beta_T \int_\Omega \hat{m}_T \left[-\Delta m_T + \int_0^T \nabla u \cdot \nabla p \, dt\right] dx + \int_\Gamma \beta_T \hat{m}_T \nabla m_T \cdot n \, ds$$

arbitrary in Ω arbitrary on Γ

$\Rightarrow$

$$\boxed{\mathcal{G}_T(m) = -\beta_T \Delta m_T + \int_0^T \nabla u \cdot \nabla p \quad \text{in } \Omega \qquad \left(\text{and } \beta_T \frac{\partial m_T}{\partial n} \text{ on } \Gamma\right)}$$

Notice this resembles the gradient for the steady-state advection diffusion equation, except that the $\nabla u \cdot \nabla p$ term is integrated over time.

The gradient w.r.t m_I is found as:

$\delta_{m_I} \mathcal{L} = 0 \quad \forall\, m_I \in H^1 \Rightarrow$ weak form of gradient w.r.t m_I:

$$\boxed{(\mathcal{G}_I(m), \hat{m}_I) := \beta_I \int_\Omega \nabla m_I \cdot \nabla \hat{m}_I \, dx - \int_\Omega \rho c\, p(x,0)\, \hat{m}_I \, dx \quad \forall\, \hat{m}_I \in H^1}$$

where we have made use of the fact that $q = \rho c\, p(x,0)$ in Ω. The strong form is then found by arguing that $\hat{m}_I$ is arbitrary in Ω:

$$\boxed{\mathcal{G}_I(m) := -\beta_I \Delta m_I + \rho c\, p(x,0) \quad \text{in } \Omega \quad \left(\text{and } \beta_I \frac{\partial m_I}{\partial n} \text{ on } \Gamma\right)}$$

So in place of the term $\int_0^T \nabla u \cdot \nabla p$ that appears in the expression for the gradient with respect to m_T, here we have simply the value of the adjoint $p(x,0)$, which is the ending value of $p(x,t)$ after we have integrated backward in time.

The Hessian can be derived similarly.