

## Supplementary Material: Mathematical Deductions

### Learning PDEs for Image Restoration via Optimal Control

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### 1 Optimal Control Governed by Evolutionary PDEs

We present the related mathematical deductions of our L-PDE model. Our learning framework is based on the following PDE-constrained optimization problem:

$$\min_{\mathbf{a}} J(\{u_k\}_{k=1}^K, \mathbf{a}), \quad s.t. \begin{cases} \frac{\partial u_k}{\partial t} = L(u_k, \mathbf{a}), & (x, y, t) \in Q, \\ u_k = 0, & (x, y, t) \in \Gamma, \\ u_k|_{t=0} = f_k, & (x, y) \in \Omega, \end{cases} \quad (1)$$

where

$$J(\{u_k\}_{k=1}^K, \mathbf{a}) = \frac{1}{2} \sum_{k=1}^K \int_{\Omega} (u_k(T_f) - \tilde{u}_k)^2 d\Omega + \frac{1}{2} \sum_{i=0}^5 \alpha_i \int_0^{T_f} a_i^2(t) dt. \quad (2)$$

The above problem can be solved if we can find the Gâteaux derivative of  $J(\{u_k\}_{k=1}^K, \mathbf{a})$  with respect to  $\mathbf{a}$ , as in this case the optimal  $\mathbf{a}$  can be computed by using the conjugate gradient.

Here we introduce the following adjoint approach to provide an efficient solution to the Gâteaux derivative.

The Lagrangian function of problem (1) is:

$$\begin{aligned} \tilde{J}(\{u_k\}_{k=1}^K, \mathbf{a}; \{\varphi_k\}_{k=1}^K) \\ = J(\{u_k\}_{k=1}^K, \mathbf{a}) + \sum_{k=1}^K \int_Q \varphi_k [(u_k)_t - L(u_k, \mathbf{a})] dQ, \end{aligned} \quad (3)$$

where  $\varphi_k$  are the adjoint functions.

To find the adjoint equations for  $\varphi_k$ , we perturb  $L$  with respect to  $u$ . The perturbation can be written as follows:

$$\begin{aligned} & L(u + \varepsilon \cdot \delta u) - L(u) \\ &= \varepsilon \cdot \left( \frac{\partial L(u)}{\partial u}(\delta u) + \frac{\partial L(u)}{\partial u_x} \frac{\partial \delta u}{\partial x} + \dots + \frac{\partial L(u)}{\partial u_{yy}} \frac{\partial^2(\delta u)}{\partial y^2} \right) + o(\varepsilon) \\ &= \varepsilon \sum_{(p,q) \in \wp} \frac{\partial L(u)}{\partial u_{pq}} \frac{\partial^{p+q}(\delta u)}{\partial x^p \partial y^q} + o(\varepsilon) \\ &= \varepsilon \sum_{(p,q) \in \wp} \sigma_{pq}(u) \frac{\partial^{p+q}(\delta u)}{\partial x^p \partial y^q} + o(\varepsilon). \end{aligned} \quad (4)$$

Then we have

$$\begin{aligned} \delta \tilde{J}_{u_k} &= \tilde{J}(\dots, u_k + \varepsilon \cdot \delta u_k, \dots) - \tilde{J}(\dots, u_k, \dots) \\ &= \varepsilon \int_{\Omega} (u_k(T_f) - \tilde{u}_k) \delta u_k(T_f) d\Omega \\ &\quad + \varepsilon \int_Q \varphi_k(\delta u_k)_t dQ - \varepsilon \int_Q \varphi_k \sum_{(p,q) \in \wp} \sigma_{pq}(u_k) \frac{\partial^{p+q}(\delta u_k)}{\partial x^p \partial y^q} dQ. \end{aligned} \quad (5)$$

As the perturbation  $\delta u_k$  should satisfy  $\delta u_k|_{\Gamma} = 0$  and  $\delta u_k|_{t=0} = 0$ , due to the boundary and initial conditions of  $u_k$ , integrating by parts, the integration on the boundary  $\Gamma$  will vanish. So we have

$$\begin{aligned} & \delta \tilde{J}_{u_k} \\ &= \varepsilon \int_{\Omega} (u_k(T_f) - \tilde{u}_k) \delta u_k(T_f) d\Omega + \varepsilon \int_{\Omega} (\varphi_k \cdot \delta u_k)(T_f) d\Omega \\ &\quad - \varepsilon \int_Q (\varphi_k)_t \delta u_k dQ - \varepsilon \int_Q \sum_{(p,q) \in \wp} (-1)^{(p+q)} \frac{\partial^{p+q}(\sigma_{pq}(u_k) \varphi_k)}{\partial x^p \partial y^q} \delta u_k dQ + o(\varepsilon) \\ &= \varepsilon \int_Q \left[ (\varphi_k + u_k(T_f) - \tilde{u}_k) \delta(t - T_f) \right. \\ &\quad \left. - (\varphi_k)_t - \sum_{(p,q) \in \wp} (-1)^{(p+q)} \frac{\partial^{p+q}(\sigma_{pq}(u_k) \varphi_k)}{\partial x^p \partial y^q} \right] \delta u_k dQ + o(\varepsilon). \end{aligned} \quad (6)$$

So the adjoint equation for  $\varphi_k$  is

$$\begin{cases} \frac{\partial \varphi_k}{\partial t} + \sum_{(p,q) \in \wp} (-1)^{(p+q)} \frac{\partial^{p+q}(\sigma_{pq}(u_k) \varphi_k)}{\partial x^p \partial y^q} = 0, & (x, y, t) \in Q, \\ \varphi_k = 0, & (x, y, t) \in \Gamma, \\ \varphi_k|_{t=T_f} = \tilde{u}_k - u_k(T_f), & (x, y) \in \Omega, \end{cases} \quad (7)$$

in order to make  $\frac{d\tilde{J}}{du_k} = 0$ .

The difference in  $\tilde{J}$  caused by perturbing  $a_i$  is

$$\begin{aligned}
\delta \tilde{J}_{a_i} &= \tilde{J}(\dots, a_i + \varepsilon \cdot \delta a_i, \dots) - \tilde{J}(\dots, a_i, \dots) \\
&= \frac{1}{2} \alpha_i \int_0^{T_f} (a_i + \varepsilon \cdot \delta a_i)^2(t) dt - \frac{1}{2} \alpha_i \int_0^{T_f} a_i^2(t) dt \\
&\quad - \sum_{k=1}^K \int_Q \varphi_k [(a_i + \varepsilon \cdot \delta a_i)(t) - a_i(t)] \text{inv}_i(u_k) dQ \\
&= \varepsilon \int_0^{T_f} (\alpha_i a_i \cdot \delta a_i)(t) dt - \varepsilon \int_0^{T_f} \left( \sum_{k=1}^K \int_\Omega \varphi_k \text{inv}_i(u_k) d\Omega \right) \delta a_i dt.
\end{aligned} \tag{8}$$

Thus we have

$$\frac{d\tilde{J}}{da_i} = \alpha_i a_i - \sum_{k=1}^K \int_\Omega \varphi_k \text{inv}_i(u_k) d\Omega, \quad i = 0, \dots, 5. \tag{9}$$