

GRADIENTS AND NONLINEAR LEAST SQUARES

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1. Introduction

We consider the dynamical system

$$y'(t) = F(t, y(t), p), \quad y(0) = y_0 \quad (1.1)$$

where F is a mapping from $\mathbf{R} \times \mathbf{R}^N \times \mathbf{R}^M$ to \mathbf{R}^N .

2. Full Measurement

We suppose y is known, call it y^\sharp on some interval, $[0, T]$, and we ask how to recover the parameter set, p^\sharp , that gave rise to this y^\sharp . We do this by solving

$$\min_{p \in \mathbf{R}^M} J(p), \quad J(p) \equiv \int_0^T \|y(t; p) - y^\sharp(t)\|^2 dt \quad (2.1)$$

where $y(t; p)$ is the solution to (1.1) for the current choice of p . Our interest here is in effective ways of computing the gradient of the objective function, J , in (2.1).

We consider the Lagrangian

$$L(y, z, p) \equiv \int_0^T \|y(t) - y^\sharp(t)\|^2 dt + \int_0^T z(t) \cdot (y'(t) - F(t, y(t), p)) dt \quad (2.2)$$

and trust in the fact that

$$J(p) = \min_y \max_z L(y, z, p)$$

and so look for critical points, in y and z , of L . To begin, the directional derivative

$$L_y(y, z, p) \cdot \tilde{y} = 2 \int_0^T (y(t) - y^\sharp(t)) \cdot \tilde{y}(t) dt + \int_0^T z(t) \cdot (\tilde{y}' - F_y(t, y(t), p)\tilde{y}(t)) dt$$

after integration by parts brings

$$L_y(y, z, p) \cdot \tilde{y} = 2 \int_0^T (y(t) - y^\sharp(t)) \cdot \tilde{y}(t) dt + z(T) \cdot \tilde{y}(T) - \int_0^T (z'(t) + F_y^*(t, y(t), p)z(t)) \cdot \tilde{y}(t) dt$$

As this must vanish for each \tilde{y} it follows that z must obey the terminal value problem

$$z'(t) + F_y^*(t, y(t), p)z(t) = 2(y(t) - y^\sharp(t)), \quad z(T) = 0. \quad (2.3)$$

With y and z in hand one may proceed to compute

$$J_p(p) \cdot \tilde{p} = L_p(y, z, p) \cdot \tilde{p} = - \int_0^T z(t) \cdot F_p(t, y(t), p)\tilde{p} dt$$

Let us apply this in the case that

$$F(t, y, p) = \begin{pmatrix} p_1 y_1 + p_2 y_1 y_2 \\ p_3 y_1 + p_4 y_2 \end{pmatrix}$$

One easily finds

$$F_y(t, y(t), p) = \begin{pmatrix} p_1 + p_2 y_2 & p_2 y_1 \\ p_3 & p_4 \end{pmatrix} \quad \text{and} \quad F_p(t, y(t), p) = \begin{pmatrix} y_1 & y_1 y_2 & 0 & 0 \\ 0 & 0 & y_1 & y_2 \end{pmatrix}$$

3. Spiky Data

In situations with rapid transients it can be useful to use a J of the form

$$J(p) \equiv \int_0^T \|Y(t; p) - Y^\sharp(t)\|^2 dt$$

where Y is the running integral of y , i.e.,

$$Y(t; p) \equiv \int_0^t y(s; p) ds.$$

Now the leading term in the y derivative of the associated Lagrangian is

$$2 \int_0^T (\mu(T) - \mu(t)) \cdot \tilde{y}(t) dt$$

where

$$\mu(t) \equiv \int_0^t (t - s)(y(s) - y^\sharp(s)) ds$$

4. Pointwise Measurement

In the case that we only measure the state at the specific times, $\{t_k\}_{k=1}^K$, our objective function takes the form

$$J(p) \equiv \sum_{k=1}^K \|y(t_k; p) - y^\sharp(t_k)\|^2 = \int_0^T \sum_{k=1}^K \|y(t; p) - y^\sharp(t)\|^2 \delta(t - t_k) dt$$

Now all that changes is the righthand side of the adjoint equation. Namely, we must solve

$$z'(t) + F_y^*(t, y(t), p)z(t) = 2(y(t) - y^\sharp(t)) \sum_{k=1}^K \delta(t - t_k), \quad z(T) = 0. \quad (4.1)$$

This is, in fact, a sequence of simple problems between the measurement times. First,

$$\begin{aligned} z'(t; K) + F_y^*(t, y(t), p)z(t; K) &= 0, \quad t_{K-1} < t < t_K, \\ z(t_K; K) &= 2(y^\sharp(t_K) - y(t_K)) \end{aligned}$$

next

$$\begin{aligned} z'(t; K-1) + F_y^*(t, y(t), p)z(t; K-1) &= 0, \quad t_{K-2} < t < t_{K-1}, \\ z(t_{K-1}; K-1) &= z(t_{K-1}; K) - 2(y(t_{K-1}) - y^\sharp(t_{K-1})) \end{aligned}$$

and in this fashion until

$$\begin{aligned} z'(t; 1) + F_y^*(t, y(t), p)z(t; 1) &= 0, \quad 0 < t < t_1, \\ z(t_1; 1) &= z(t_1; 2) - 2(y(t_1) - y^\sharp(t_1)) \end{aligned}$$