IC-32 **Optimal Control** Spring 2009

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Problem Set #10

1. The objective of this problem is to calculate, by **three different numerical methods**, the gradient of a functional

$$\mathcal{F}(\mathbf{p}) := \phi(\mathbf{x}(t_\mathrm{f}), \mathbf{p}), \tag{1}$$

where $\mathbf{p} \in \mathbb{R}^{n_p}$ is a set of time-invariant parameters, and the state variables $\mathbf{x}(t) \in \mathbb{R}^{n_x}$ are the solutions of an initial value problem (IVP)

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{p}); \qquad \mathbf{x}(t_0) = \mathbf{h}(\mathbf{p}). \tag{2}$$

The functions ϕ, $\mathbf{f}$ and $\mathbf{h}$ are assumed to be continuously differentiable with respect to all their argument throughout.

For each $i = 1, \ldots, n_p$, estimates of the gradient can be calculated as follows:

- Finite differences approach:

$$\boldsymbol{\nabla}_{p_i}\mathcal{F}(\mathbf{p}) \approx \frac{\mathcal{F}(p_1, \ldots, p_i + \delta p_i, \ldots, p_{n_p}) - \mathcal{F}(\mathbf{p})}{\delta p_i}; \tag{3}$$

- Forward sensitivity approach:

$$\boldsymbol{\nabla}_{p_i}\mathcal{F}(\mathbf{p}) = \phi_{\mathbf{x}}(\mathbf{x}(t_\mathrm{f}), \mathbf{p})\ \mathbf{x}_{p_i}(t_\mathrm{f}) + \phi_{p_i}(\mathbf{x}(t_\mathrm{f}), \mathbf{p}) \tag{4}$$

$$\text{with:}\quad \dot{\mathbf{x}}_{p_i}(t) = \mathbf{f}_{\mathbf{x}}(t, \mathbf{x}(t), \mathbf{p})\ \mathbf{x}_{p_i}(t) + \mathbf{f}_{p_i}(t, \mathbf{x}(t), \mathbf{p}); \qquad \mathbf{x}_{p_i}(t_0) = \mathbf{h}_{p_i}(\mathbf{p}); \tag{5}$$

- Adjoint (reverse) sensitivity approach:

$$\boldsymbol{\nabla}_{p_i}\mathcal{F}(\mathbf{p}) = \phi_{p_i}(\mathbf{x}(t_\mathrm{f}), \mathbf{p}) + q_i(t_0) + \boldsymbol{\lambda}(t_0)^\mathsf{T}\mathbf{h}_{p_i}(\mathbf{p}) \tag{6}$$

$$\text{with:}\quad \dot{\boldsymbol{\lambda}}(t) = -\mathbf{f}_{\mathbf{x}}(t, \mathbf{x}(t), \mathbf{p})^\mathsf{T}\boldsymbol{\lambda}(t); \qquad \boldsymbol{\lambda}(t_\mathrm{f}) = \phi_{\mathbf{x}}(\mathbf{x}(t_\mathrm{f}), \mathbf{p}) \tag{7}$$

$$\dot{q}_i(t) = -\mathbf{f}_{p_i}(t, \mathbf{x}(t), \mathbf{p})^\mathsf{T}\boldsymbol{\lambda}(t); \qquad q_i(t_\mathrm{f}) = 0. \tag{8}$$

As an application, we shall consider the problem of a batch reactor doing the degradation of a substrate S by a biomass X, according to the auto-catalyzed reaction $S \to X$. The differential equations for the system are simply:

$$\dot{S}(t) = -\mu(S)X \tag{9}$$

$$\dot{X}(t) = \frac{1}{Y}\mu(S)X, \tag{10}$$

where the rate of reaction $\mu(S)$ is given by

$$\mu(S) = \mu_M \frac{S}{K+S}.$$

The parameter and initial concentration values are $Y = 0.75$, $K = 10$, $\mu_M = 0.1$, $S(0) = 5$, and $X(0) = 10$.

(a) In MATLAB®, calculate the concentration of biomass $X(t_f)$ at $t_f = 10$, by solving the ODEs (9,10).

(b) Using the finite difference approach, estimate the gradient of $X(t_f)$ with respect to the parameter μ_M and the initial concentration of biomass $X(0)$. In particular, try out different values for the perturbation parameter δp_i in (3)

(c) Write down the sensitivity equations (5) corresponding to (9,10), for the sensitivity parameters taken as μ_M and $X(0)$. In MATLAB®, solve the resulting equations, along with (9,10), and then calculate the gradient of $X(t_f)$ with respect to μ_M and $X(0)$ based on (4).

(d) Write down the adjoint equations (7,8) corresponding to (9,10). In MATLAB®, solve the resulting equations backward in time, by interpolating the state variables, and then calculate the gradient of $X(t_f)$ with respect to μ_M and $X(0)$ based on (6).

INDICATIONS:

- Use the function `ode15s` to integrate the differential equations (set both the absolute and relative integration tolerances to 10^{-6});
- In the adjoint approach, use the function `interp1` to interpolate the values of the state variables (use the option '`spline`' of `interp1`).

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2. In this exercise, we consider the problem to find a minimizing control for the Bolza-type functional

$$\int_{t_0}^{t_f} \ell(t, \mathbf{x}, \mathbf{u})\, dt + \phi(\mathbf{x}(t_f)), \tag{11}$$

subject to

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}, \mathbf{u}); \quad \mathbf{x}(t_0) = \mathbf{x}_0, \tag{12}$$

where $\mathbf{u} \in \mathcal{C}[t_0, t_f]$, and both the initial time t_0 and the terminal time t_f are fixed. It shall be supposed throughout that ℓ and $\mathbf{f}$ are continuous in $(t, \mathbf{x}, \mathbf{u})$ and have continuous first partial derivatives with respect to $\mathbf{x}$ and $\mathbf{u}$, for all $(t, \mathbf{x}, \mathbf{u}) \in [t_0, t_f] \times \mathbb{R}^{n_x} \times \mathbb{R}^{n_u}$; ϕ is continuous and has continuous first partial derivatives with respect to $\mathbf{x}$, for all $\mathbf{x} \in \mathbb{R}^{n_x}$.

(a) Prove that, if $\mathbf{u}^\star \in \mathcal{C}[t_0, t_f]^{n_u}$ is a (local) minimizer for (11,12), with response $\mathbf{x}^\star \in \mathcal{C}^1[t_0, t_f]^{n_x}$, then there is a function $\boldsymbol{\lambda}^\star \in \mathcal{C}^1[t_0, t_f]^{n_x}$ such that the triple $(\mathbf{u}^\star, \mathbf{x}^\star, \boldsymbol{\lambda}^\star)$ satisfies the system

$$\dot{\mathbf{x}}(t) = \mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t)); \qquad \mathbf{x}(t_0) = \mathbf{x}_0 \tag{13}$$

$$\dot{\boldsymbol{\lambda}}(t) = -\ell_{\mathbf{x}}(t, \mathbf{x}(t), \mathbf{u}(t)) - \mathbf{f}_{\mathbf{x}}(t, \mathbf{x}(t), \mathbf{u}(t))^{\mathsf{T}} \boldsymbol{\lambda}(t); \qquad \boldsymbol{\lambda}(t_f) = \boldsymbol{\phi}_{\mathbf{x}}(\mathbf{x}(t_f) \tag{14}$$

$$\mathbf{0} = \ell_{\mathbf{u}}(t, \mathbf{x}(t), \mathbf{u}(t)) + \mathbf{f}_{\mathbf{u}}(t, \mathbf{x}(t), \mathbf{u}(t))^{\mathsf{T}} \boldsymbol{\lambda}(t). \tag{15}$$

for $t_0 \leq t \leq t_f$.
Hint: Use similar arguments to the proof of Theorem 4.9 in the class textbook.

(b) Justify the adjoint terminal condition $\boldsymbol{\lambda}^\star(t_f) = \boldsymbol{\phi}_{\mathbf{x}}(\mathbf{x}(t_f))$ in light of the discussion help in §4.4.4 of the class textbook.

(c) **Application:** Consider the optimal control problem

$$\text{minimize:} \quad \int_0^1 [x(t) - u(t)] \, \mathrm{d}t + x(1) \tag{16}$$

$$\text{subject to:} \quad \dot{x}(t) \;=\; 1 + [u(t)]^2; \quad x(0) \;=\; 1. \tag{17}$$

i. Find candidate solutions to the problem (16,17) based on the first-order necessary conditions developed above.

ii. Check that the Hamiltonian function $\mathcal{H} = \ell + \boldsymbol{\lambda}^\mathsf{T}\mathbf{f}$ is constant along the candidate optimal solution(s).

(d) Let $(\mathbf{u}^\star, \mathbf{x}^\star, \boldsymbol{\lambda}^\star)$ be a solution to the Euler-Lagrange equations (13–15). Prove that for $\mathbf{u}^\star$ to be a global minimizer to (11,12), it is sufficient that:

(i) ℓ and $\mathbf{f}$ be jointly convex in $(\mathbf{u}, \mathbf{x})$, for each $(t, \mathbf{u}, \mathbf{x}) \in [t_0, t_\mathrm{f}] \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_x}$;

(ii) ϕ be convex in $\mathbf{x}$, for each $\mathbf{x} \in \mathbb{R}^{n_x}$; and

(iii) $\boldsymbol{\lambda}^\star(t) \geq \mathbf{0}$ (component-wise), for each $t \in [t_0, t_\mathrm{f}]$.

Hint: Use similar arguments to the proof of Theorem 4.11 in the class textbook.

(e) **Application:** What can be said about the candidate optimal control(s) found previously for the problem (16,17)?