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Problem Set #10 (With Solutions)

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

$$\mathcal{F}(\mathbf{p}) := \phi(\mathbf{x}(t_f), \mathbf{p}), \quad (1)$$

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)

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

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

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

- o Finite differences approach:

$$\nabla_{p_i} \mathcal{F}(\mathbf{p}) \approx \frac{\phi(\mathbf{x}(t_f), p_1, \dots, p_i + \delta p_i, \dots, p_{n_p}) - \phi(\mathbf{x}(t_f), \mathbf{p})}{\delta p_i}; \quad (3)$$

- o Forward sensitivity approach:

$$\nabla_{p_i} \mathcal{F}(\mathbf{p}) = \phi_{\mathbf{x}}(\mathbf{x}(t_f), \mathbf{p}) \mathbf{x}_{p_i}(t_f) + \phi_{p_i}(\mathbf{x}(t_f), \mathbf{p}) \quad (4)$$

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

- o Adjoint (reverse) sensitivity approach:

$$\nabla_{p_i} \mathcal{F}(\mathbf{p}) = \phi_{p_i}(\mathbf{x}(t_f), \mathbf{p}) + z_i(t_0) + \boldsymbol{\lambda}(t_0)^\top \mathbf{h}_{p_i}(\mathbf{p}) \quad (6)$$

$$\text{with: } \dot{\boldsymbol{\lambda}}(t) = -\mathbf{f}_{\mathbf{x}}(t, \mathbf{x}(t), \mathbf{p})^\top \boldsymbol{\lambda}(t); \quad \boldsymbol{\lambda}(t_f) = \phi_{\mathbf{x}}(\mathbf{x}(t_f), \mathbf{p}) \quad (7)$$

$$\dot{z}_i(t) = -\mathbf{f}_{p_i}(t, \mathbf{x}(t), \mathbf{p})^\top \boldsymbol{\lambda}(t); \quad z_i(t_f) = 0. \quad (8)$$

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 $S \rightarrow X$. The differential equations for the system are simply:

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

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

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).

Solution. A possible implementation is as follows:

```

main.m
1  clear all;
2  clf;
3  format long;
4
5  % Options for ODE solver
6  opt = odeset( 'RelTol', 1e-6, 'AbsTol', 1e-6 );
7
8  % Parameters
9  t0 = 0;
10 tf = 10;
11 muM = 0.1;
12 K = 10;
13 R = 0.75;
14 S0 = 5;
15 X0 = 10;
16
17 % Forward state integration: t0 -> tf
18 [tx,yx] = ode23s(@(t,y)syst(t,y,muM,K,R), [t0,tf], [S0,X0], opt);
19 Xf=yx(end,2);
20 disp(sprintf('Biomass concentration at final time: %d', Xf));

```

```

syst.m
1  function [dy] = syst( t, y, muM, K, R )
2      % State equations
3      mu = muM * y(1) / ( K + y(1) );
4      dy = [ - mu * y(2);
5             mu / R * y(2) ];
6  end

```

With this implementation, the concentration of biomass at final time is found to be

$$X(10) \approx 13.9876.$$

- (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).

Solution. A possible implementation is as follows (with the same function `syst.m` as before):

```

main.m
1  clear all;
2  clf;
3  format long;
4
5  % Options for ODE solver
6  opt = odeset( 'RelTol', 1e-6, 'AbsTol', 1e-6 );
7
8  % Parameters
9  t0 = 0;
10 tf = 10;

```

```

11 muM = 0.1;
12 K = 10;
13 R = 0.75;
14 S0 = 5;
15 X0 = 10;
16
17 % Forward state integration: t0 -> tf, with default parameters
18 [tx,yx] = ode23s(@(t,y)syst(t,y,muM,K,R), [t0,tf], [S0,X0], opt);
19 Xf=yx(end,2);
20 disp(sprintf('Biomass concentration at final time: %d', Xf));
21
22 %Forward Finite Differences Approach (for various perturbations)
23 for iexp = -3:-2:-9
24     tol = 10^iexp;
25     disp(sprintf('\nFinite Differences Approach (Perturbation: %d):', tol));
26
27     % Forward state integration: t0 -> tf, with perturbed muM
28     muMp = muM*(1+tol);
29     [tx,yx] = ode23s(@(t,y)syst(t,y,muMp,K,R), [t0,tf], [S0,X0], opt);
30     Xfper=yx(end,2);
31     dXf_FD(1) = (Xfper-Xf)/(muMp-muM);
32     disp(sprintf('Sens. of biomass concentration at final time w.r.t. muM: %d',...
33                 dXf_FD(1)));
34
35     % Forward state integration: t0 -> tf, with perturbed x0
36     X0p = X0*(1+tol);
37     [tx,yx] = ode23s(@(t,y)syst(t,y,muM,K,R), [t0,tf], [S0,X0p], opt);
38     Xfper=yx(end,2);
39     dXf_FD(2) = (Xfper-Xf)/(X0p-X0);
40     disp(sprintf('Sens. of biomass concentration at final time w.r.t. X0: %d',...
41                 dXf_FD(2)));
42 end
43

```

With the foregoing implementation, one gets the following results:

Perturbation	$X_{\mu_M}(10)$	$X_{X_0}(10)$
10^{-3}	31.19419	1.260091
10^{-5}	31.20564	1.260203
10^{-7}	31.20575	1.260205
10^{-9}	31.20670	1.260228

For the specified integration tolerances (10^{-6}), a suitable perturbation magnitude appears to be in the order of 10^{-5} – 10^{-7} . That is, approximate sensitivity values for the biomass concentration at final time with respect to μ_M and X_0 are as follows:

$$X_{\mu_M}(10) \approx 31.2057, \quad X_{X_0}(10) \approx 1.26020.$$

Next, we shall confirm these values based on forward and reverse sensitivity analyses.

- (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).

Solution. The sensitivity equations for the model (9,10) with respect to μ_M and $X(0)$ are

given by:

$$\begin{aligned}\dot{S}_{\mu_M}(t) &= -\mu_S(S(t)) X(t) S_{\mu_M}(t) - \mu(S(t)) X_{\mu_M}(t) - \mu_{\mu_M}(S(t)) X(t); & S_{\mu_M}(0) &= 0 \\ \dot{X}_{\mu_M}(t) &= \frac{1}{Y} [\mu_S(S(t)) X(t) S_{\mu_M}(t) + \mu(S(t)) X_{\mu_M}(t) + \mu_{\mu_M}(S(t)) X(t)]; & X_{\mu_M}(0) &= 0\end{aligned}$$

$$\begin{aligned}\dot{S}_{X_0}(t) &= -\mu_S(S(t)) X(t) S_{X_0}(t) - \mu(S(t)) X_{X_0}(t); & S_{X_0}(0) &= 0 \\ \dot{X}_{X_0}(t) &= \frac{1}{Y} [\mu_S(S(t)) X(t) S_{X_0}(t) + \mu(S(t)) X_{X_0}(t)]; & X_{X_0}(0) &= 1\end{aligned}$$

with:

$$\begin{aligned}\mu_S(S) &= \mu_M \frac{K}{(K+S)^2} \\ \mu_{\mu_M}(S) &= \frac{S}{K+S}.\end{aligned}$$

An implementation of the forward sensitivity approach is given subsequently. Observe that the sensitivity equations are integrated, forward in time, along with the state equations.

```

----- main.m -----
1  clear all;
2  clf;
3  format long;
4
5  % Options for ODE solver
6  opt = odeset( 'RelTol', 1e-6, 'AbsTol', 1e-6 );
7
8  % Parameters
9  t0 = 0;
10 tf = 10;
11 muM = 0.1;
12 K = 10;
13 R = 0.75;
14 S0 = 5;
15 X0 = 10;
16
17 % Forward state/sensitivity integration: t0 -> tf
18 [ts,ys] = ode23s(@(t,y)sens(t,y,muM,K,R), [t0,tf], [S0,X0,0,0,0,1], opt);
19
20 % Results
21 disp(sprintf('\nForward Sensitivity Approach:'));
22 dXf_FS(1) = ys(end,4);
23 disp(sprintf('Sens. of biomass concentration at final time w.r.t. muM: %d',...
24             dXf_FS(1)));
25 dXf_FS(2) = ys(end,6);
26 disp(sprintf('Sens. of biomass concentration at final time w.r.t. X0: %d',...
27             dXf_FS(2)));
----- sens.m -----
1  function [dy] = sens( t, y, muM, K, R )
2  % State & sensitivity equations
3  mu = muM * y(1) / ( K + y(1) );
4  dmudmuM = y(1) / ( K + y(1) );
5  dmudS = muM * K / ( K + y(1) )^2;
6  dy = [ -mu * y(2);
7         mu / R * y(2);

```

```

8      - dmudS * y(2) * y(3) - mu * y(4) - dmudmuM * y(2);
9      dmudS * y(2) / R * y(3) + mu / R * y(4) + dmudmuM / R * y(2);
10     - dmudS * y(2) * y(5) - mu * y(6);
11     dmudS * y(2) / R * y(5) + mu / R * y(6) ];
12     end

```

With the foregoing implementation, one gets the following results:

$$X_{\mu_M}(10) \approx 31.20519, \quad X_{X_0}(10) \approx 1.260201,$$

which are rather close to those obtained via finite differences.

- (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).

Solution. In the reverse mode of sensitivity analysis, the sensitivity values for the biomass concentration at final time with respect to μ_M and X_0 are obtained as:

$$\begin{aligned} X_{\mu_M}(10) &= z_{\mu_M}(0) \\ X_{X_0}(10) &= \lambda_X(0), \end{aligned}$$

where the adjoint equations for the model (9,10) are given by:

$$\begin{aligned} \dot{\lambda}_S(t) &= \mu_S(S(t)) X(t) \left(\lambda_S(t) - \frac{1}{Y} \lambda_X(t) \right); & \lambda_S(10) &= 0 \\ \dot{\lambda}_X(t) &= \mu(S(t)) \left(\lambda_S(t) - \frac{1}{Y} \lambda_X(t) \right); & \lambda_X(10) &= 1 \\ \dot{z}_{\mu_M}(t) &= \mu_{\mu_M}(S(t)) X(t) \left(\lambda_S(t) - \frac{1}{Y} \lambda_X(t) \right); & z_{\mu_M}(10) &= 0. \end{aligned}$$

with the functions $\mu_S(\cdot)$ and $\mu_{\mu_M}(\cdot)$ defined earlier. Note also that $z_{X_0}(t) = 0, \forall t$, so the corresponding differential equation has been omitted.

An implementation of the adjoint sensitivity approach is given subsequently. Observe that the state equations are integrated first, forward in time; then, the adjoint equations are integrated, backward in time, using interpolated values for the state variables.

```

main.m
1     clear all;
2     clf;
3     format long;
4
5     % Options for ODE solver
6     opt = odeset( 'RelTol', 1e-6, 'AbsTol', 1e-6 );
7
8     % Parameters
9     t0 = 0;
10    tf = 10;
11    muM = 0.1;
12    K = 10;
13    R = 0.75;
14    S0 = 5;
15    X0 = 10;
16
17    % Forward state integration: t0 -> tf

```

```

18 [tx,yx] = ode23s(@(t,y)syst(t,y,muM,K,R), [t0,tf], [S0,X0], opt);
19
20 % Backward adjoint integration: tf -> t0
21 [ta,ya] = ode23s(@(t,y)adj(t,y,muM,K,R,tx,yx), [tf,t0], [0,1,0], opt);
22
23 % Results
24 disp(sprintf('\n Reverse (Adjoint) Sensitivity Approach'));
25 dXf_AS(1) = ya(end,3);
26 disp(sprintf('Sens. of biomass concentration at final time w.r.t. muM: %d',...
27             dXf_AS(1)));
28 dXf_AS(2) = ya(end,2);
29 disp(sprintf('Sens. of biomass concentration at final time w.r.t. X0: %d',...
30             dXf_AS(2)));

```

```

----- adj.m -----
1 function [dy] = adj( t, y, muM, K, R, tspan, xspan )
2 % Calculate the states [S,X] at current time t by interpolation
3 x = interp1( tspan, xspan(:,1:2), t, 'spline' );
4 % Adjoint equations
5 mu = muM * x(1) / ( K + x(1) );
6 dmudmuM = x(1) / ( K + x(1) );
7 dmudS = muM * K / ( K + x(1) )^2;
8 dy = [ dmudS * x(2) * ( y(1) - 1 / R * y(2) );
9       mu * ( y(1) - 1 / R * y(2) );
10      dmudmuM * x(2) * ( y(1) - 1 / R * y(2) ) ];
11 end

```

With the foregoing implementation, the following sensitivity values are obtained:

$$X_{\mu_M}(10) \approx 31.20510, \quad X_{X_0}(10) \approx 1.260200,$$

which are again close to those obtained via forward sensitivity analysis as well as finite differences.

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`).

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

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

subject to

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

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

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

$$\dot{\boldsymbol{\lambda}}(t) = -\ell_{\mathbf{x}}(t, \mathbf{x}(t), \mathbf{u}(t)) - \mathbf{f}_{\mathbf{x}}(t, \mathbf{x}(t), \mathbf{u}(t))^{\top} \boldsymbol{\lambda}(t); \quad \boldsymbol{\lambda}(t_f) = \phi_{\mathbf{x}}(\mathbf{x}(t_f)) \quad (14)$$

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

for $t_0 \leq t \leq t_f$.

[Hint: Use similar arguments to the proof of Theorem 3.9 in the class textbook.]

Solution. Consider a one-parameter family of comparison controls $\mathbf{v}(t; \eta) := \mathbf{u}^*(t) + \eta \boldsymbol{\omega}(t)$, where $\boldsymbol{\omega}(t) \in \mathcal{C}[t_0, t_f]^{n_u}$ is some fixed function, and η is a (scalar) parameter. Based on the continuity and differentiability properties of \mathbf{f} , we know that there exists $\bar{\eta} > 0$ such that the response $\mathbf{y}(t; \eta) \in \mathcal{C}^1[t_0, t_f]^{n_x}$ associated to $\mathbf{v}(t; \eta)$ through (12) exists, is unique, and is differentiable with respect to η , for all $\eta \in \mathcal{B}_{\bar{\eta}}(0)$ and for all $t \in [t_0, t_f]$. Clearly, $\eta = 0$ provides the optimal response $\mathbf{y}(t; 0) \equiv \mathbf{x}^*(t)$, $t_0 \leq t \leq t_f$.

Since the control $\mathbf{v}(t; \eta)$ is admissible and its associated response is $\mathbf{y}(t; \eta)$, we have

$$\begin{aligned} \mathcal{J}(\mathbf{v}(t; \eta)) &= \int_{t_0}^{t_f} \left[\ell(t, \mathbf{y}(t; \eta), \mathbf{v}(t; \eta)) + \boldsymbol{\lambda}(t)^{\top} [\mathbf{f}(t, \mathbf{y}(t; \eta), \mathbf{v}(t; \eta)) - \dot{\mathbf{y}}(t; \eta)] \right] dt + \phi(\mathbf{y}(t_f; \eta)) \\ &= \int_{t_0}^{t_f} \left[\ell(t, \mathbf{y}(t; \eta), \mathbf{v}(t; \eta)) + \boldsymbol{\lambda}(t)^{\top} \mathbf{f}(t, \mathbf{y}(t; \eta), \mathbf{v}(t; \eta)) + \dot{\boldsymbol{\lambda}}(t)^{\top} \mathbf{y}(t; \eta) \right] dt \\ &\quad - \boldsymbol{\lambda}(t_f)^{\top} \mathbf{y}(t_f; \eta) + \boldsymbol{\lambda}(t_0)^{\top} \mathbf{y}(t_0; \eta) + \phi(\mathbf{y}(t_f; \eta)), \end{aligned}$$

for any $\boldsymbol{\lambda} \in \mathcal{C}^1[t_0, t_f]^{n_x}$ and for each $\eta \in \mathcal{B}_{\bar{\eta}}(0)$. Based on the differentiability properties of ℓ , ϕ , and \mathbf{y} , we have

$$\begin{aligned} \frac{\partial}{\partial \eta} \mathcal{J}(\mathbf{v}(t; \eta)) &= \int_{t_0}^{t_f} \left[\ell_{\mathbf{u}}(t, \mathbf{y}(t; \eta), \mathbf{v}(t; \eta)) + \mathbf{f}_{\mathbf{u}}(t, \mathbf{y}(t; \eta), \mathbf{v}(t; \eta))^{\top} \boldsymbol{\lambda}(t) \right]^{\top} \boldsymbol{\omega}(t) dt \\ &\quad + \int_{t_0}^{t_f} \left[\ell_{\mathbf{x}}(t, \mathbf{y}(t; \eta), \mathbf{v}(t; \eta)) + \mathbf{f}_{\mathbf{x}}(t, \mathbf{y}(t; \eta), \mathbf{v}(t; \eta))^{\top} \boldsymbol{\lambda}(t) + \dot{\boldsymbol{\lambda}}(t) \right]^{\top} \mathbf{y}_{\eta}(t; \eta) dt \\ &\quad + [\phi_{\mathbf{x}}(\mathbf{y}(t_f; \eta)) - \boldsymbol{\lambda}(t_f)]^{\top} \mathbf{y}_{\eta}(t_f; \eta) + \boldsymbol{\lambda}(t_0)^{\top} \mathbf{y}_{\eta}(t_0; \eta), \end{aligned}$$

for any $\boldsymbol{\omega} \in \mathcal{C}[t_0, t_f]^{n_u}$ and any $\boldsymbol{\lambda} \in \mathcal{C}^1[t_0, t_f]^{n_x}$. Taking the limit as $\eta \rightarrow 0$, and since $\mathbf{y}_{\eta}(t_0; \eta) = 0$, we get

$$\begin{aligned} \delta \mathcal{J}(\mathbf{u}^*; \boldsymbol{\omega}) &= \int_{t_0}^{t_f} \left[\ell_{\mathbf{u}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t)) + \mathbf{f}_{\mathbf{u}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t))^{\top} \boldsymbol{\lambda}(t) \right]^{\top} \boldsymbol{\omega}(t) dt \\ &\quad + \int_{t_0}^{t_f} \left[\ell_{\mathbf{x}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t)) + \mathbf{f}_{\mathbf{x}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t))^{\top} \boldsymbol{\lambda}(t) + \dot{\boldsymbol{\lambda}}(t) \right]^{\top} \mathbf{y}_{\eta}(t; 0) dt \\ &\quad + [\phi_{\mathbf{x}}(\mathbf{x}^*(t_f)) - \boldsymbol{\lambda}(t_f)]^{\top} \mathbf{y}_{\eta}(t_f; 0), \end{aligned}$$

which is finite for each $\boldsymbol{\omega} \in \mathcal{C}[t_0, t_f]^{n_u}$ and each $\boldsymbol{\lambda} \in \mathcal{C}^1[t_0, t_f]^{n_x}$, since the integrand is continuous on $[t_0, t_f]$. That is, $\delta \mathcal{J}(\mathbf{u}^*; \boldsymbol{\omega})$ exists for each $\boldsymbol{\omega} \in \mathcal{C}[t_0, t_f]^{n_u}$ and each $\boldsymbol{\lambda} \in \mathcal{C}^1[t_0, t_f]^{n_x}$.

Since \mathbf{u}^* is a local minimizer, we get

$$0 = \int_{t_0}^{t_f} \left[\ell_{\mathbf{x}}^* + \mathbf{f}_{\mathbf{x}}^{\top} \boldsymbol{\lambda}(t) + \dot{\boldsymbol{\lambda}}(t) \right]^{\top} \mathbf{y}_{\eta}(t; 0) + \left[\ell_{\mathbf{u}}^* + \mathbf{f}_{\mathbf{u}}^{\top} \boldsymbol{\lambda}(t) \right]^{\top} \boldsymbol{\omega}(t) dt + [\phi_{\mathbf{x}}^* - \boldsymbol{\lambda}|_{t=t_f}^{\top}]^{\top} \mathbf{y}_{\eta}(t_f; 0),$$

for each $\boldsymbol{\omega} \in \mathcal{C}[t_0, t_f]^{n_u}$ and each $\boldsymbol{\lambda} \in \mathcal{C}^1[t_0, t_f]^{n_x}$; where the compressed notations $\ell_z^* := \ell_z(t, \mathbf{x}^*(t), \mathbf{u}^*(t))$, $\mathbf{f}_z^* := \mathbf{f}_z(t, \mathbf{x}^*(t), \mathbf{u}^*(t))$, and $\phi_z^* = \phi_z(\mathbf{x}^*(t_f))$ are used.

Because the effect of a variation of the control on the course of the response is hard to determine (i.e., $\mathbf{y}_{\eta}(t; 0)$), we choose $\boldsymbol{\lambda}^*(t)$, $t_0 \leq t \leq t_f$, so as to obey the differential equation

$$\dot{\boldsymbol{\lambda}}(t) = -\mathbf{f}_{\mathbf{x}}^{\top} \boldsymbol{\lambda}(t) - \ell_{\mathbf{x}}^*, \quad (16)$$

with the terminal condition

$$\boldsymbol{\lambda}(t_f) = \phi_{\mathbf{x}}^*.$$

Note that (16) being a linear system of ODEs, and from the regularity assumptions on ℓ and \mathbf{f} , the solution $\boldsymbol{\lambda}^*$ exists and is unique over $[t_0, t_f]$, i.e., $\boldsymbol{\lambda} \in \mathcal{C}^1[t_0, t_f]^{n_x}$. That is, the condition

$$0 = \int_{t_0}^{t_f} \left[\ell_{\mathbf{u}}^* + \mathbf{f}_{\mathbf{u}}^{*\top} \boldsymbol{\lambda}^*(t) \right]^\top \boldsymbol{\omega}(t) dt,$$

must hold for any $\boldsymbol{\omega} \in \mathcal{C}[t_0, t_f]^{n_u}$. In particular, for $\boldsymbol{\omega}(t) := \ell_{\mathbf{u}}^* + \mathbf{f}_{\mathbf{u}}^{*\top} \boldsymbol{\lambda}^*(t)$, we get

$$0 = \int_{t_0}^{t_f} \left[\ell_{\mathbf{u}}^* + \mathbf{f}_{\mathbf{u}}^{*\top} \boldsymbol{\lambda}^*(t) \right]^2 dt,$$

which, in turn, implies the necessary condition that

$$0 = \ell_{\mathbf{u}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t)) + \mathbf{f}_{\mathbf{u}}(t, \mathbf{x}^*(t), \mathbf{u}^*(t))^\top \boldsymbol{\lambda}^*(t),$$

for each $t \in [t_0, t_f]$.

- (b) Justify the adjoint terminal condition $\boldsymbol{\lambda}^*(t_f) = \phi_{\mathbf{x}}(\mathbf{x}(t_f))$ in light of the discussion help in §3.4.4 of the class textbook.

Solution. We saw in §3.4.4 of the class textbook that $\boldsymbol{\lambda}^*(t)$, $t_0 \leq t \leq t_f$, can be interpreted as the rate of change of the optimal cost value if the state of the system were slightly perturbed at time t . Here, it is easy to see that the integral part of the optimal cost value would *not* change if the state at t_f were slightly perturbed. On the other hand, the terminal term would be modified as

$$\phi(\mathbf{x}^*(t_f) + \delta\mathbf{x}(t_f)) = \phi(\mathbf{x}^*(t_f)) + \phi_{\mathbf{x}}(t_f, \mathbf{x}(t_f))^\top \delta\mathbf{x}(t_f) + o(\delta\mathbf{x}(t_f)).$$

That is, the first variation $\delta\mathcal{J}$ in the optimal cost value would be

$$\delta\mathcal{J} = \phi_{\mathbf{x}}(\mathbf{x}^*(t_f))^\top \delta\mathbf{x}(t_f),$$

This interpretation thus confirms the terminal adjoint condition

$$\boldsymbol{\lambda}^*(t_f) = \phi_{\mathbf{x}}(\mathbf{x}^*(t_f)).$$

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

$$\text{minimize: } \int_0^1 [x(t) - u(t)] dt + x(1) \tag{17}$$

$$\text{subject to: } \dot{x}(t) = 1 + [u(t)]^2; \quad x(0) = 1. \tag{18}$$

- i. Find candidate solutions to the problem (17,18) based on the first-order necessary conditions developed above.

Solution. We start by forming the Hamiltonian function

$$\mathcal{H}(x, u, \lambda) = x - u + \lambda(1 + u^2).$$

Necessary conditions of optimality are given by (18) and

$$\begin{aligned} \dot{x}(t) &= \mathcal{H}_x = 1 + [u(t)]^2; & x(0) &= 1 \\ \dot{\lambda}^*(t) &= -\mathcal{H}_x = -1; & \lambda^*(1) &= \phi_{\mathbf{x}} = 1 \\ 0 &= \mathcal{H}_u = -1 + 2\lambda^*u^*. \end{aligned}$$

The adjoint equation is trivially integrated as

$$\lambda^*(t) = 2 - t,$$

and from the stationarity condition $\mathcal{H}_u = 0$, we get

$$u^*(t) = \frac{1}{2(2-t)}.$$

(Note that u^* is indeed a candidate *minimum* solution for the problem since $\mathcal{H}_{uu} = 2(2-t) > 0$ for each $0 \leq t \leq 1$.) Finally, substituting the optimal control candidate back into (18) yields

$$\dot{x}^*(t) = 1 + \frac{1}{4(2-t)^2}; \quad x(0) = 1.$$

Integrating this last equation, and drawing the results together, we obtain

$$u^*(t) = \frac{1}{2(2-t)} \tag{19}$$

$$x^*(t) = t + \frac{1}{4(2-t)} + \frac{7}{8} \tag{20}$$

$$\lambda^*(t) = 2 - t. \tag{21}$$

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

Solution. Since the problem is autonomous (neither ℓ nor \mathbf{f} depend explicitly on t), the Hamiltonian function should be constant along (u^*, x^*, λ^*) . Here, it is easily established that

$$\mathcal{H}(x^*(t), u^*(t), \lambda^*(t)) = \frac{23}{8},$$

for each $t \in [0, 1]$.

- (d) Let $(\mathbf{u}^*, \mathbf{x}^*, \boldsymbol{\lambda}^*)$ be a solution to the Euler-Lagrange equations (13–15). Prove that for \mathbf{u}^* 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 $(t, \mathbf{u}, \mathbf{x}) \in [t_0, t_f] \times \mathbb{R}^{n_u} \times \mathbb{R}^{n_x}$;
- (ii) ϕ be convex in \mathbf{x} , for each $\mathbf{x} \in \mathbb{R}^{n_x}$; and
- (iii) $\boldsymbol{\lambda}^*(t) \geq \mathbf{0}$ (component-wise), for each $t \in [t_0, t_f]$.

[Hint: Use similar arguments to the proof of Theorem 3.11 in the class textbook.]

Solution. Provided that conditions (i) and (ii) hold, for any feasible control $\mathbf{u}(t)$ and its associated response $\mathbf{x}(t)$, we have

$$\begin{aligned} \mathcal{J}(\mathbf{u}) - \mathcal{J}(\mathbf{u}^*) &= \int_{t_0}^{t_f} [\ell(t, \mathbf{x}(t), \mathbf{u}(t)) - \ell(t, \mathbf{x}^*(t), \mathbf{u}^*(t))] dt + [\phi(\mathbf{x}(t_f)) - \phi(\mathbf{x}^*(t_f))] \\ &\geq \int_{t_0}^{t_f} \left(\ell_{\mathbf{x}}^{*\top} [\mathbf{x}(t) - \mathbf{x}^*(t)] + \ell_{\mathbf{u}}^{*\top} [\mathbf{u}(t) - \mathbf{u}^*(t)] \right) dt + \phi_{\mathbf{x}}^{*\top} [\mathbf{x}(t_f) - \mathbf{x}^*(t_f)], \end{aligned}$$

with the usual compressed notation. Since the triple $(\mathbf{u}^*, \mathbf{x}^*, \boldsymbol{\lambda}^*)$ satisfies the Euler-Lagrange equations (13–15), we obtain

$$\begin{aligned} \mathcal{J}(\mathbf{u}) - \mathcal{J}(\mathbf{u}^*) &\geq \int_{t_0}^{t_f} \left(-[\mathbf{f}_{\mathbf{x}}^{*\top} \boldsymbol{\lambda}^*(t) + \dot{\boldsymbol{\lambda}}^*(t)]^\top [\mathbf{x}(t) - \mathbf{x}^*(t)] - [\mathbf{f}_{\mathbf{u}}^{*\top} \boldsymbol{\lambda}^*(t)]^\top [\mathbf{u}(t) - \mathbf{u}^*(t)] \right) dt \\ &\quad + \phi_{\mathbf{x}}^{*\top} [\mathbf{x}(t_f) - \mathbf{x}^*(t_f)], \end{aligned}$$

Integrating by part the term in $\dot{\lambda}^*(t)$, and rearranging the terms, we get

$$\begin{aligned} \mathcal{J}(\mathbf{u}) - \mathcal{J}(\mathbf{u}^*) &\geq \int_{t_0}^{t_f} \lambda^*(t)^\top (\mathbf{f}(t, \mathbf{x}(t), \mathbf{u}(t)) - \mathbf{f}(t, \mathbf{x}^*(t), \mathbf{u}^*(t)) - \mathbf{f}_x^* [\mathbf{x}(t) - \mathbf{x}^*(t)] - \mathbf{f}_u^* [\mathbf{u}(t) - \mathbf{u}^*(t)]) dt \\ &\quad + [\phi_x^* - \lambda^*(t_f)]^\top [\mathbf{x}(t_f) - \mathbf{x}^*(t_f)] + \lambda^*(t_0)^\top [\mathbf{x}(t_0) - \mathbf{x}^*(t_0)]. \end{aligned}$$

Note that the integrand is positive provided that conditions (i) and (iii) hold; the remaining two terms are equal to zero due to the optimal adjoint boundary conditions and the prescribed state initial conditions, respectively, in the Euler-Lagrange equations. That is,

$$\mathcal{J}(\mathbf{u}) \geq \mathcal{J}(\mathbf{u}^*),$$

for each feasible control if conditions (i), (ii), and (iii) hold.

- (e) **Application:** What can be said about the candidate optimal control(s) found previously for the problem (17,18)?

Solution. The integrand term is linear (and thus convex) in (u, x) , the salvage term is also linear with respect to x , and the right-hand side of the differential equation (18) is (strictly) convex in u (and independent of x). Moreover, the (unique) solution (19,21) to the Euler-Lagrange equations (13–15) is such that

$$\lambda^*(t) := 2 - t \geq 0,$$

for each $t \in [0, 1]$. We can therefore conclude that $u^*(t) := \frac{1}{2(2-t)}$, $0 \leq t \leq 1$, is a (global) optimal control for the problem (17,18).
