Pontryagin's Maximum Principle in Optimal Control

$$\dot{x} = f(x,u) \qquad x(t) \in \mathbb{R}^n, \quad u(t) \in \mathbb{R}^m$$

Optimal control problem:

$\min J(T,0,x,u(\cdot))$ over "admissible" controls $u(\cdot)$

where $J(T,t,x,u(\cdot)) := \int_t^T q(x(s),u(s))\,ds + r(x(T))$

$$\text{s.t.} \quad \dot{x}(s) = f(x(s),u(s)) \qquad t \le s \le T$$
$$x(t) = x$$

Admissible controls: $\varphi_1(u(t)) \le 0, \dots, \varphi_r(u(t)) \le 0 \quad \forall t \in [0,T]$

- **Reduction to the Mayer problem**

$$\dot{x}_i = f_i(x_1,\dots,x_n,u) \qquad i=1,\dots,n$$
$$\dot{x}_{n+1} = q(x_1,\dots,x_n,u)$$
$$\dot{x}_{n+2} = \sum_{i=1}^n \frac{\partial}{\partial x_i} r(x_1,\dots,x_n) f_i(x_1,\dots,x_n,u)$$

s.t. $x_1(0) = x_1, \dots, x_n(0) = x_n$

$x_{n+1}(0) = 0$

$x_{n+2}(0) = r(x_1,\dots,x_n)$

$$\min_{u(\cdot)} J(T,0,x,u(\cdot)) \longrightarrow \boxed{\min_{u(\cdot)} x_{n+1}(T) + x_{n+2}(T)}$$

b/c $x_{n+1}(T) = \int_0^T q(x_1(t),\dots,x_n(t),u(t))\,dt$

$x_{n+2}(T) = r(x_1(T),\dots,x_n(T))$

Bottom line: no loss of generality if we seek $u(\cdot)$ [subject to given constraints] to minimize

$c^T x(T)$ for some fixed $c = (c_1,\dots,c_n) \in \mathbb{R}^n$.

Recap:

1) co-states: $x_i(t) \longrightarrow p_i(t)$ s.t.

$$\frac{d}{dt} p_i(t) = -\sum_{j=1}^{n} p_j(t) \frac{\partial}{\partial x_i} f_j(x_1(t), \dots, x_n(t), u(t))$$

$$p_i(T) = -c_i \qquad i = 1, \dots, n$$

2) Hamiltonian function $H : \mathbb{R}^n \times \mathbb{R}^n \times \mathbb{R}^m \to \mathbb{R}$

$$H(x, p, u) := \sum_{i=1}^{n} p_i f_i(x_1, \dots, x_n, u_1, \dots, u_m)$$

3) Then $\dot{x}_i = \frac{\partial H}{\partial p_i}$ $\qquad i \in \{1, \dots, n\}$

$$\dot{p}_i = -\frac{\partial H}{\partial x_i}$$

s.t. boundary conditions $x(0) = x$, $p(T) = -c$

4) PMP: if $\bar{u}(\cdot)$ is an optimal control strategy, then

$$H(\bar{x}(t), \bar{p}(t), \bar{u}(t)) = \max_{v_1, \dots, v_m} H(\bar{x}(t), \bar{p}(t), v)$$

over all $v = (v_1, \dots, v_m)^T$ s.t. $\varphi_1(v) \leq 0, \dots, \varphi_r(v) \leq 0$

where $(\bar{x}(t), \bar{p}(t))$ are the state/co-state trajectories induced by $\bar{u}(\cdot)$.

5) If $\bar{u}(\cdot)$ is optimal, then

$$\bar{u}(t) = K(\bar{x}(t), \bar{p}(t))$$

where
$$K(x, p) := \underset{\substack{u_1, \dots, u_m \\ \varphi_1(u) \leq 0 \\ \dots \\ \varphi_r(u) \leq 0}}{\arg\max} H(x, p, u);$$

then
$$\dot{\bar{x}}(t) = f(\bar{x}(t), K(\bar{x}(t), \bar{p}(t)))$$
$$\dot{\bar{p}}(t) = -\bar{p}(t) \frac{\partial}{\partial x} f(\bar{x}(t), K(\bar{x}(t), \bar{p}(t)))$$

s.t. $\bar{x}(0)=x$, $\bar{p}(T) = -c^T$

6) If $V(t,x) := \min_{u(\cdot)} J(T,t,x,u(\cdot))$

where $J(T,t,x,u(\cdot)) = c^T x(T)$

then $\bar{p}_i(t) = -\frac{\partial}{\partial x_i} V(t,x)\Big|_{x=\bar{x}(t)}$ ...

(connection to Dynamic Programming)

<u>Example</u> (scalar LQR)

$$\dot{x} = ax + bu \qquad x, u \in \mathbb{R}$$

$$\min_{u(\cdot)} \frac{1}{2}\int_0^T (ru^2 + qx^2)\,dx \qquad r>0,\ q \geq 0$$

Define x_1, x_2: $\quad x_1(t) = x(t)$

$\quad x_2(t) = \frac{1}{2}\int_0^t (ru^2(s) + qx^2(s))\,ds$

$$\dot{x}_1 = ax_1 + bu$$

$$\dot{x}_2 = \frac{1}{2}qx_1^2 + \frac{1}{2}ru^2 \qquad x_2(0)=0$$

$$\min_{u(\cdot)} x_2(T) \equiv \min_{u(\cdot)} (0,\ 1)\begin{pmatrix} x_1(T) \\ x_2(T) \end{pmatrix} \qquad c = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$H(x_1, x_2, p_1, p_2, u) = p_1(ax_1 + bu) + p_2\left(\frac{1}{2}qx_1^2 + \frac{1}{2}ru^2\right)$$

$$= ap_1x_1 + \frac{1}{2}qp_2x_1^2 + \frac{1}{2}rp_2u^2 + bp_1u$$

$$\dot{p}_1 = -\frac{\partial H}{\partial x_1} = -ap_1 - qp_2x_1$$

$$\dot{p}_2 = -\frac{\partial H}{\partial x_2} = 0 \qquad \Rightarrow \qquad p_2(t) = -1$$

$\Rightarrow H(x_1, x_2, p_1, p_2, u)$ $\qquad p_2(t) = -1$

$= a p_1 x_1 - \frac{1}{2} q x_1^2 - \frac{1}{2} r u^2 + b p_1 u$

$\frac{\partial H}{\partial u} = -ru + bp_1 = 0 \qquad K(x_1, x_2, p_1, p_2) = \frac{b}{r} p_1$

Closed-loop dynamics:

$\dot{x}_1 = a x_1 + \frac{b^2}{r} p_1 \qquad x_1(0) = x_1$

$\dot{p}_1 = -a p_1 + q x_1 \qquad p_1(T) = 0$

- can integrate this and obtain optimal control.

<u>Interpretation of the Co-State</u>

$\dot{x} = f(x, u)$

$\dot{p} = -p \frac{\partial}{\partial x} f(x, u)$ $\qquad$ s.t. bd conditions

$H(x(t), p(t), u(t)) = p(t)\, \dot{x}(t)$

- projection of $\dot{x}(t)$ onto the costate $p(t)$

<u>Claim A</u>: $p_i(t) = -\frac{\partial}{\partial x_i} J(T, t, x(t), u(\cdot))$

where $J(T, t, x, u(\cdot)) = c^T x(T)$

when $\dot{x}(s) = f(x(s), u(s))$, $T \geq s \geq t$
$x(t) = x$

Bd cond. $(t = T)$: $\frac{\partial}{\partial x_i} J(T, T, x, u(\cdot)) = c_i$

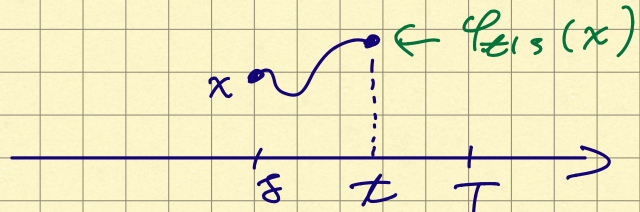
<u>Proof</u> $\quad \dot{x}(t) = f(t, x(t))$

[think $f(t, x(t)) \equiv f(x(t), u(t))$ for a chosen $u(\cdot)$]

Flow: $\varphi_{t,s}(x)$ $\qquad 0 \le s \le t \le T$

$$\frac{d}{dt}\varphi_{t,s}(x) = f(t, \varphi_{t,s}(x)) \qquad T \geq t \geq s$$

$$\varphi_{s,s}(x) = x$$



Let $J : \mathbb{R}^n \to \mathbb{R}$ be given (w/ suitable regularity)

$$J_{T,t}(x) := J(\underbrace{\varphi_{T,t}(x)}_{x(T)}) \quad \text{when } x(t) = x$$

$$p(t) := -\frac{\partial}{\partial x} J_{T,t}(x)\Big|_{x = x(t)}$$

$$p(T) = -\frac{\partial}{\partial x} J_{T,T}(x) = -\frac{\partial J}{\partial x}(x(T)) \in \mathbb{R}^{1\times n}$$

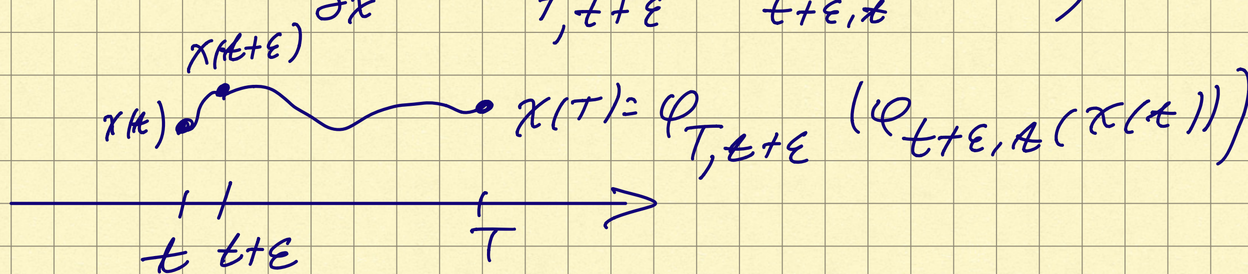
<u>Claim B:</u> $\frac{d}{dt} p(t) = -p(t) \frac{\partial}{\partial x} f(t, x(t))$

s.t. $p(T) = -\frac{\partial J}{\partial x}(x(T))$

$$p(t) = -\frac{\partial}{\partial x}(J \circ \varphi_{T,t})(x(t))$$

$$= -\frac{\partial}{\partial x} J(\varphi_{T,t}(x(t)))$$

$$= -\frac{\partial}{\partial x} J(\varphi_{T,t+\varepsilon}(\varphi_{t+\varepsilon,t}(x(t))))$$



Chain rule: $\frac{\partial}{\partial x} J(\varphi_{T,t+\varepsilon}(\varphi_{t+\varepsilon,t}(x(t))))$

$$= \underbrace{\frac{\partial}{\partial x}\left(J\circ\varphi_{T,t+\varepsilon}\right)\Big(\underbrace{\varphi_{t+\varepsilon,t}(x(t))}_{x(t+\varepsilon)}\Big)}_{\frac{\partial}{\partial x}J\left(\varphi_{T,t+\varepsilon}(x(t+\varepsilon))\right)}\frac{\partial}{\partial x}\varphi_{t+\varepsilon,t}(x(t))$$

$$= -p(t+\varepsilon)\,\frac{\partial}{\partial x}\varphi_{t+\varepsilon,t}(x(t))$$

$$\therefore \quad \boxed{p(t) = p(t+\varepsilon)\,\frac{\partial}{\partial x}\varphi_{t+\varepsilon,t}(x(t))}$$

$$\frac{p(t+\varepsilon)-p(t)}{\varepsilon} = \frac{1}{\varepsilon}\,p(t+\varepsilon)\left(I_n - \frac{\partial}{\partial x}\varphi_{t+\varepsilon,t}(x(t))\right)$$

$$= -p(t+\varepsilon)\cdot\frac{1}{\varepsilon}\left(\frac{\partial}{\partial x}\varphi_{t+\varepsilon,t}(x(t)) - I_n\right)$$

$\lim\limits_{\varepsilon\downarrow 0}(\cdots)$:

$$\frac{d}{dt}p(t) = -p(t)\lim_{\varepsilon\downarrow 0}\frac{1}{\varepsilon}\left(\frac{\partial}{\partial x}\varphi_{t+\varepsilon,t}(x(t)) - I_n\right)$$

$$= -p(t)\,\frac{\partial}{\partial x}f(t,x(t)), \qquad p(T) = -\frac{\partial}{\partial x}J(x(T))$$

$$\varphi_{t+\varepsilon,t}(x) = x + \varepsilon f(t,x) + o(\varepsilon)$$

$$\frac{\partial}{\partial x}\varphi_{t+\varepsilon,t}(x) = I_n + \varepsilon\frac{\partial}{\partial x}f(t,x) + o(\varepsilon)$$

$$\frac{1}{\varepsilon}\left\{\frac{\partial}{\partial x}\varphi_{t+\varepsilon,t}(x) - I_n\right\} = \frac{\partial}{\partial x}f(t,x) + \frac{o(\varepsilon)}{\varepsilon}$$

$$\xrightarrow{\varepsilon\downarrow 0} \frac{\partial}{\partial x}f(t,x).$$

Bottom Line: $p(t)$ (co-state) measures the sensitivity of the cost-to-go at time t to $x(t)$

Implications:

1) Sensitivity of dynamical systems to parameter perturbations

$\dot{x}(t) = f(x(t); \theta)$ $\qquad x(t) \in \mathbb{R}^n$, $\theta \in \mathbb{R}^k$ (parameters)

$a_{ij}(t) := \frac{\partial}{\partial \theta_j} x_i(t)$

$x(t) \longrightarrow \begin{pmatrix} x(t) \\ z(t) \end{pmatrix}$, $\quad z(t) \in \mathbb{R}^k$

$$\begin{aligned} \dot{x} &= f(x, z) & x(0) &= x \\ \dot{z} &= 0 & z(0) &= \theta \end{aligned}$$

Cost : $x_i(T) = c^T \begin{pmatrix} x(T) \\ z(T) \end{pmatrix} = \begin{pmatrix} e_i & \vdots & 0 \end{pmatrix} \begin{pmatrix} x(T) \\ z(T) \end{pmatrix}$

then you can compute $a_{ij}(t)$ as the appropriate coordinate of the co-state

2) Computation of gradients in ML

deep neural nets:

$x(l+1) = F(x(l), \theta(l))$

$x(0)$ - input
$x(l)$ - activation of layer l
$\theta(l)$ - weights at layer l

special case:

$F(x, \theta) = x + \underset{\text{small}}{\underset{\downarrow}{\varepsilon}} f(x, \theta)$ $\qquad$ (Residual Network, a.k.a ResNet)

Ex. 10: $\underbrace{\dot{x}(t) = f(x(t), \theta(t))}$ $\hookrightarrow$ $\theta(\cdot)$ - control

$$\min_{\theta(\cdot)} c^T x(T)$$ [reduction to Mayer cost assumed]

$\to$ Neural ODE (Chen et al., 2018 NeurIPS)
$[\theta(t) = \theta(0)]$

$$\frac{\partial}{\partial \theta_i} c^T x(T; \theta)$$ – can be carried out using co-state evolution