Automatic Control and Biosystem

Optimal Microalgal Growth Problem

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Proposition

Let u^{opt} be optimal control minimizing the performance index J, given as:

$$\dot{x} = f(x,u), x = [x_1, \ldots, x_n]^\top \in \mathrm{R}^n, u \in U \subset \mathrm{R}^m,$$
$$J = \int_{t_0}^{t_f} f_0(x,u)\mathrm{d}t + \phi(x(t_f)),\ x(t_0) = x^0,\ x(t_f) \in \mathrm{R}^n,$$

where $x^0 \in \mathrm{R}^n, 0 \le t_0 < t_f$ and compact U are given and let $x^{opt}(t), x^{opt}(0) = x^0$, is the corresponding state trajectory. Then $\exists \psi(t) = [\psi_1(t), \ldots, \psi_n(t)]^\top \not\equiv 0$ such that it holds $\forall t \in [t_0, t_f]$:

$$\dot{\psi} = \frac{\partial f_0}{\partial x}(u^{opt}, x^{opt})^\top - \frac{\partial f}{\partial x}(u^{opt}, x^{opt})^\top \psi, \quad \psi^\top(t_f) = -\frac{\partial \phi}{\partial x}(x(t_f)),$$

$$\max_{u \in U} \Big[-f_0(x^{opt}(t), u) + \psi^\top(t) f(x^{opt}(t), u) \Big] =$$
$$\Big[-f_0(x^{opt}(t), u^{opt}(t)) + \psi^\top(t) f(x^{opt}(t), u^{opt}(t)) \Big].$$

Pontryagin maximum principle

Problem with free terminal condition and fixed time interval

Without any loss of generality one can put $\phi \equiv 0$, as

$$\phi(x(t_f)) = \phi(x_0) + \int_{t_0}^{t_f} \frac{\partial \phi}{\partial x}\dot{x}\mathrm{d}t = \phi(x_0) + \int_{t_0}^{t_f} \frac{\partial \phi}{\partial x} f(x,u)\mathrm{d}t,$$

and as $\phi(x_0)$ is uniquely given, it is sufficient to replace $f_0(x,u)$ by $\widetilde{f}_0(x,u) := f_0(x,u) + \frac{\partial \phi}{\partial x} f(x,u)$

and co-state $\psi(t)$, $\psi(t_f) = -\frac{\partial \phi}{\partial x}(x(t_f))$ by new co-state $\widetilde{\psi}(t) := \psi + \frac{\partial \phi}{\partial x}(t)$, $\widetilde{\psi}(t_f) = 0$, due to the following:

$$\dot{\widetilde{\psi}} = \dot{\psi} + \frac{\partial^2 \phi}{\partial x^2} f(x,u) = \frac{\partial^2 \phi}{\partial x^2} f(x,u) + \frac{\partial f_0}{\partial x}(u^{opt}, x^{opt})^\top - \frac{\partial f}{\partial x}(u^{opt}, x^{opt})^\top \widetilde{\psi}$$
$$+ \frac{\partial \phi}{\partial x}(t) \frac{\partial f}{\partial x}(u^{opt}, x^{opt})^\top = \frac{\partial \widetilde{f}_0}{\partial x}(u^{opt}, x^{opt})^\top - \frac{\partial f}{\partial x}(u^{opt}, x^{opt})^\top \widetilde{\psi}.$$

Pontryagin maximum principle

Problem with free terminal condition and fixed time interval

Equivalent problem:

for given t_0, t_f, x^0, U, *find* $T_0 < T_f \in \mathrm{R}$ *and measurable* $u^{opt}(t) \in U, t \in [T_0, T_f]$, *which minimizes* $x_0(T_f)$, *where:*

$$\dot{x}_0 = f_0(x,u),\ \dot{x} = f(x,u),\ \dot{x}_{n+1} = 1,\ \ [x_0, x, x_{n+1}](T_0) = (0, x^0, t_0),$$
$$[x_0, x, x_{n+1}](T_f) \in \{\tilde{x} = [\tilde{x}_0, \tilde{x}, \tilde{x}_{n+1},] \in \mathrm{R}^{n+2} \mid \tilde{x}_{n+1} = t_f\}.$$

We use formulation of Pontryagin maximum principle (PMP) from [PBGM] *Pontrjagin, Boltjanskij, Gamkrelidze, Miščenko: Mathematical Theory of Control Processes*[1].

[1] 1961, Fizmatgiz, R; 1962, Wiley, E; 1964, Praha, SNTL, CZ; 1964, Pergamon Press, E; 1964 Berlin, Dt. Verl. Wiss., G; 1966, Tokyo, J; 1967 Wien and Munich, G; 1968 Warzsava, P; 1969 Moscow, Nauka, 2nd Ed., R; 1976 3rd, R; 1983 4th, R; 1978 Moscow, Nauka, F.

Pontryagin maximum principle

Problem with free terminal condition and fixed time interval

By basic theorem in [PBGM] optimality of $u^{opt}(t) \in U, t \in [T_0, T_f]$, with free $T_0 < T_f$ implies the existence of $\overline{\psi}(t) \not\equiv 0$, where

$$(1)\quad \dot{\psi}_0 = 0,\ \dot{\psi} = -\left[\frac{\partial f_0}{\partial x}\right]^\top \psi_0 - \left[\frac{\partial f}{\partial x}\right]^\top \psi,\ \dot{\psi}_{n+1} = 0$$

$$(2)\quad \overline{\psi} := [\psi_0, \psi, \psi_{n+1}]^\top,\ \psi(T_f) = 0,$$

such that it holds

$$(3)\quad H(\overline{\psi}(t), u^{opt}(t), x^{opt}(t)) = \max_{u \in U} H(\overline{\psi}(t), u, x^{opt}(t))$$

$$(4)\quad \psi_0(T_f) \le 0,\ H(\overline{\psi}(T_f), u^{opt}(T_f), x^{opt}(T_f)) = 0,$$

$H := \psi_0 f_0 + \psi^\top f + \psi_{n+1}$ - Hamiltonian of the extended system.

Pontryagin maximum principle

Problem with free terminal condition and fixed time interval

By (2) one has that conditions (4) are equivalent

$$\psi_{n+1}(T_f) + \psi_0(T_f) f_0(T_f) = 0, \; \psi_0(T_f) \le 0,$$

Since $\psi_0(T_f) = 0 \Rightarrow \overline{\psi}(t) \equiv 0$, contradicts PMP, it must even hold by (1,2) that

(5) $\psi_{n+1}(T_f) + \psi_0(T_f) f_0(T_f) = 0, \; \psi_0(T_f) < 0,$

Since $\psi_0(T_f) < 0$, equality in (5) can by fullfilled choosing proper $\psi_{n+1}(T_f)$.

By homogeneity of the co-state equation (1) and Hamiltonian $H := \psi_0 f_0 + \psi^\top f + \psi_{n+1}$ wrt $\overline{\psi} = [\psi_0, \psi, \psi_{n+1}]^\top$, it has to exist the solution with $\psi_0(T_f) = -1 \Rightarrow \psi_0(t) \equiv -1$ as well.

Then, conditions (1,2,3,4) are granted by conditions of Proposition.

Model of microalgal growth and its properties

Chlorella vulgaris

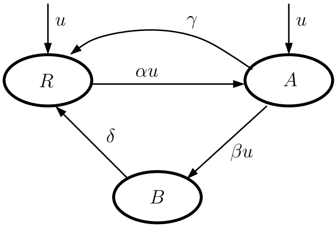

Figure: Eilers-Peeters model of photosynthesis.

"A" activated state;
"B" inhibitated state;
"R" resting state.

Model of microalgal growth and its properties

Let x_A, x_B, x_R, $x_A + x_B + x_R = 1$, be probabilities, or relative concentrations of the corresponding states, x_A, x_B directly measurable.

(6)
$$\begin{bmatrix} \dot{x_A} \\ \dot{x_B} \end{bmatrix} = \begin{bmatrix} -\gamma & 0 \\ 0 & -\delta \end{bmatrix} \begin{bmatrix} x_A \\ x_B \end{bmatrix} + u(t) \begin{bmatrix} -(\alpha+\beta) & -\alpha \\ \beta & 0 \end{bmatrix} \begin{bmatrix} x_A \\ x_B \end{bmatrix} + u(t) \begin{bmatrix} \alpha \\ 0 \end{bmatrix},$$

(7) $$J = \kappa\gamma(t_f - t_0)^{-1} \int_{t_0}^{t_f} x_A(t)\mathrm{d}t\ .$$

(8) $$x_{Ass} = \alpha\delta u \lambda_F^{-1}\lambda_S^{-1}, \quad x_{Bss} = \alpha\beta u^2 \lambda_F^{-1}\lambda_S^{-1}\ ,$$
here $\lambda_{F,S} < 0$ are appropriate eigenvalues of the matrix of the rhs of (6) with constant input.

(9) $$u_{opt_{ss}} = \gamma^{1/2}\delta^{1/2}\alpha^{-1/2}\beta^{-1/2}, \quad u^* := u/u_{opt_{ss}}.$$

Biological consistency of the model

Model (6) is acceptable from the biological point of view, in particular, as the region where its variables have the practical sense is forward invariant. This region is given by condition that x_A, x_B are nonnegative and their sum is less than 1, as also value $x_R = 1 - x_A - x_B$ is nonnegative. Therefore, next Proposition is important.

Proposition

Let

$$(10)\quad \Delta^1 := \left\{ [x_1, x_2]^\top \in \mathbb{R}^2 \,\middle|\, x_1 + x_2 \le 1, x_1 \ge 0, x_2 \ge 0 \right\}.$$

Then, Δ^1 is the forward invariant set of (6) for every nonegative and measurable function $u(t)$.

More suitable parameterization

Model (6-7) can be rewritten using the following reparameterization

$$q_1 := \sqrt{\frac{\gamma\delta}{\alpha\beta}}, q_2 := \sqrt{\frac{\alpha\beta\gamma}{\delta}}\frac{1}{\alpha+\beta}, q_3 := \kappa\gamma\sqrt{\frac{\alpha\delta}{\beta\gamma}}, q_4 := \alpha q_1, q_5 := \frac{\beta}{\alpha},$$

giving together with already introduced to $u^* := u/u_{opt_{ss}}$:

$$(11)\quad \begin{aligned} \frac{1}{q_4}\begin{bmatrix} \dot{x}_A \\ \dot{x}_B \end{bmatrix} &= -\begin{bmatrix} q_2(1+q_5) & 0 \\ 0 & \frac{q_5}{q_2(1+q_5)} \end{bmatrix}\begin{bmatrix} x_A \\ x_B \end{bmatrix} \\ &\quad -u^*\begin{bmatrix} (1+q_5) & 1 \\ -q_5 & 0 \end{bmatrix}\begin{bmatrix} x_A \\ x_B \end{bmatrix} + \begin{bmatrix} u^* \\ 0 \end{bmatrix}, \end{aligned}$$

$$(12)\quad J = q_2 q_3 (1+q_5)(t_f - t_0)^{-1}\int_{t_0}^{t_f} x_A(t)\mathrm{d}t\ .$$

More suitable parameterization

q_1 v μE m^{-2}s^{-1}, q_2, q_5 are unitless, q_3, q_4 in s^{-1};

q_1, q_2 - steady state properties;

q_3 influence only unit of production;

$q_1 := u_{opt_{ss}}$ ("constant" optimal control);

q_4 influenced dynamics only via overall time scaling;

q_5/q_2^2 is small parameter;

More precisely, [Rehák, Čelikovský, Papáček, 2008, TAC IEEE]:
$q_1 := 250.106\mu\text{Em}^{-2}\text{s}^{-1}$, $q_2 := 0.301591$, $q_3 := 0.000176498\text{s}^{-1}$, $q_4 := 0.483955\text{s}^{-1}$, $q_5 := 0.000298966$.

Formulas for steady states are also simpler:

$$x_{B_{ss}} = \frac{u^{*2}}{u^{*2} + u^{*}/q_2 + 1}, \; x_{A_{ss}} = \frac{u^{*}}{q_2(1+q_5)(u^{*2} + u^{*}/q_2 + 1)}.$$

Photoinhibition

Little light not good, but too much neither.

$x_{A_{ss}}(u^*)$: Haldan curve (Haldan steady state model of photosynthesis and photoinhibition; or steady state H. kinetics).

Haldan curve rises from 0 for $u^* = 0$ reaching maximum at $u^* = 1$ and then monotonously decreases to 0 at $+\infty$.

In other words, [11] (repeated bellow) is actually the dynamical model of photosynthesis and photoinhibition, called also as the model of the PSF (photosynthetic factory):

$$\frac{1}{q_4}\begin{bmatrix} \dot{x}_A \\ \dot{x}_B \end{bmatrix} = -\begin{bmatrix} q_2(1+q_5) & 0 \\ 0 & \frac{q_5}{q_2(1+q_5)} \end{bmatrix}\begin{bmatrix} x_A \\ x_B \end{bmatrix}$$

$$-u^*\begin{bmatrix} (1+q_5) & 1 \\ -q_5 & 0 \end{bmatrix}\begin{bmatrix} x_A \\ x_B \end{bmatrix} + \begin{bmatrix} u^* \\ 0 \end{bmatrix},$$

$$J = q_2 q_3 (1+q_5)(t_f - t_0)^{-1}\int_{t_0}^{t_f} x_A(t)\mathrm{d}t\ .$$

Light integration property

Experiments show, that microalgae has the capacity to integrate irradiation effect, i.e. for rapidly switching of dark and light periods its growth corresponds to an average constant irradiance.

Mathematical explanation: bilinear system, theorem on differential inclusion rhs convexification.

$$\dot{x} \in F(x) \rightarrow \text{ reachable set } X(t, x_0)$$

$$\dot{x} \in \overline{\text{conv}} F(x) \rightarrow \text{ reachable } \overline{X(t, x_0)}$$

[Čelikovský, Kybernetika, 1987 a 1988], particular estimates of precision and approximation algorithm for general BLS,

[Čelikovský *et al*, Kybernetika, 2007], estimates and approximation algorithm for PSF model.

Conclusion: PSF model reflects experimental observations.

Singular perturbation based reduction

$$\frac{1}{q_4}\begin{bmatrix}\dot{x}_A\\ \dot{x}_B\end{bmatrix} = -\begin{bmatrix} q_2(1+q_5) & 0\\ 0 & \frac{q_5}{q_2(1+q_5)}\end{bmatrix}\begin{bmatrix}x_A\\ x_B\end{bmatrix} - u^*\begin{bmatrix}(1+q_5) & 1\\ -q_5 & 0\end{bmatrix}\begin{bmatrix}x_A\\ x_B\end{bmatrix} + \begin{bmatrix}u^*\\ 0\end{bmatrix},$$

$\tau = t\frac{q_5}{q_2^2}$:

$$\frac{q_5}{q_2^2 q_4}\frac{\mathrm{d}}{\mathrm{d}\tau}\begin{bmatrix}x_A\\ x_B\end{bmatrix} = -\begin{bmatrix} q_2(1+q_5) & 0\\ 0 & \frac{q_5}{q_2(1+q_5)}\end{bmatrix}\begin{bmatrix}x_A\\ x_B\end{bmatrix} - u^*\begin{bmatrix}(1+q_5) & 1\\ -q_5 & 0\end{bmatrix}\begin{bmatrix}x_A\\ x_B\end{bmatrix} + \begin{bmatrix}u^*\\ 0\end{bmatrix},$$

$$\frac{1}{q_4}\begin{bmatrix}\frac{q_5}{q_2^2}\frac{\mathrm{d}x_A}{\mathrm{d}\tau}\\ \frac{\mathrm{d}x_B}{\mathrm{d}\tau}\end{bmatrix} = -\begin{bmatrix} q_2(1+q_5) & 0\\ 0 & \frac{q_2}{1+q_5}\end{bmatrix}\begin{bmatrix}x_A\\ x_B\end{bmatrix} - u^*\begin{bmatrix}(1+q_5) & 1\\ -q_2^2 & 0\end{bmatrix}\begin{bmatrix}x_A\\ x_B\end{bmatrix} + \begin{bmatrix}u^*\\ 0\end{bmatrix}.$$

Singular perturbation based reduction

$$(13)\quad \begin{aligned} {x_A}^S &= \frac{u^*(1-x_B^S)}{(u^*+q_2)(1+q_5)}, \\ \frac{\mathrm{d}x_B^S}{\mathrm{d}t} &= -\frac{q_4 q_5 x_B^S}{q_2(1+q_5)} + \frac{q_4 q_5 (1-x_B^S) {u^*}^2}{(1+q_5)(u^*+q_2)}. \end{aligned}$$

Proposition

Let $x(t, x^0), t \in \mathcal{I} := [t_0, t_1]$, is a solution of (11) with $x^0(t_0) = (x_A^0, x_B^0)^\top \in \Delta^1$, see (10) and let $u^*(t), t \in \mathcal{I}$ be a measurable function. Further, let for $U_{ap} \in [0,1], P > 0, D > 0, \varepsilon > 0$ and $\forall t \in \mathcal{I}$ it holds:

$$(14)\quad \begin{aligned} &\left| \frac{u^*(t)}{u^*(t)+q_2} - U_{ap} \right| \leq D, \ \left| {x_A}^0 - U_{ap} \frac{1-x_B^0}{1+q_5} \right| \leq P, \\ &t_1 - t_0 > T(\varepsilon) = (D+1)(q_2 q_4)^{-1} \log\left(\varepsilon^{-1} \tilde{K}(P - \overline{K})\right), \end{aligned}$$

Singular perturbation based reduction

Proposition

(15) $\widetilde{K} = \sqrt{2q_5^2 + 6q_5 + 5},\ \overline{K} = \max\left\{D + q_5, q_5\dfrac{(D+1)^2}{4q_2^2}\right\}.$

Suppose $q_{2,3,4,5} > 0,\ q_2 < 1$*. Then* $\exists x^S(t, \tilde{x}^0),\ \ x^S := (x_A^S, x_B^S)^\top$*, solution of (13) such that* $\forall\ \varepsilon > 0$ *and* $P > \overline{K}$ *it holds*

(16) $\|x^S(t, \tilde{x}^0) - x(t, x^0)\| < \widetilde{K}(\overline{K} + D) + \varepsilon,\ \ \forall\ t \geq t_0 + T(\varepsilon).$

Moreover, if $P \leq \overline{K}$*, then it holds*
$\|x^S(t, \tilde{x}^0) - x(t, x^0)\| < \widetilde{K}(\overline{K} + D)\ \forall t \geq t_0.$

Singular perturbation based reduction

Corollary

Suppose all asumptions of the previous Proposition hold, except U_{ap} *being replaced by piecewise constant function* $U_{ap}(t) \in [0,1]\ \forall t \in \mathcal{I}$ *such that abs. values of its jumps at discontinuities are less than* $E > 0$ *and time segments between jumps are shorter than* $\Delta T := (D+1)(q_2 q_4)^{-1}\log(2)$. *Then for* $P > \overline{K}$ *it holds* $\forall\ t \geq t_0 + T(\varepsilon)$

$$(17)\quad \|x^S(t,\tilde{x}^0) - x(t,x^0)\| < \widetilde{K}(\overline{K} + D + 2E) + \varepsilon.$$

Moreover, if $P \leq \overline{K}$, *then it holds* $\|x^S(t,\tilde{x}^0) - x(t,x^0)\| < \widetilde{K}(\overline{K} + D + 2E)\ \forall t \geq t_0$.

Singular perturbation based reduction

Singular perturbation based reduction thereby approximates well also systems with discontinuous inputs, if values of their jumps are small enough and time segments between them large enough.

Minimal allowed time between jumps ΔT is for given q_2, q_4
$\Delta T \approx (D+1)4.8\text{s}$, while $\widetilde{K} \approx 5, \overline{K} \approx \max\{D + 0.003, 0.0003\}$.

Approximation is affected by $u^*(t)/(u^*(t) + q_2)$, not directly by input $u^*(t)$.

Typical optimization courses: approx. 10^5s.

Therefore, level of approximation above is acceptable, though it does not exclude some weird optimal control course, for which it is not valid.

Optimal control of the one-dimensional reduction

(18) $J = \int_0^T (x_1 - 1)\frac{u(t)}{u(t)+L}\,\mathrm{d}t \ \mapsto \ \min, \ u(t) \in [0, U],$

(19) $\dot{x_1} = -\frac{K}{L}x_1 + \frac{(1-x_1)u^2}{u+L}K, \quad x_1(0) = x_1^0 \in [0,1],$

(20) $K := q_4 q_5 (1+q_5)^{-1}, \ L := q_2.$

(21) $\mathcal{H} = -\frac{u(x_1-1)}{u+L} + \psi_1 K\left(\frac{(1-x_1)u^2}{u+L} - \frac{1}{L}x_1\right),$

(22) $\dot{\psi}_1 = \frac{u}{u+L} + \psi_1\left(\frac{K}{L} + u\frac{u}{u+L}K\right), \quad \psi_1(T) = 0.$

(23) $u^o(t) = \alpha(\psi_1(t)), \alpha(\psi_1) = \min\left\{-L + \sqrt{L^2 - \frac{L}{K\psi_1}}, U\right\},$
where $\psi_1(t)$ is the solution of (22) with $u = \alpha(\psi_1)$.

Optimal control of the one-dimensional reduction

Proposition

Optimal control (23) grows on $[0, T - T^{sat}]$*, while on* $[T - T^{sat}, T]$ *it holds* $u(t) \equiv U$*. Moreover, the lenght of the saturated part* T^{sat} *does not depend on* T*, moreover*

$$T^{sat} = \frac{L(U+L)}{K(U+L+LU^2)} \log\left(\frac{U^2(U+2L)}{(U^2-1)(U+L)}\right).$$

Optimal control does not depend on initial state.

Proposition

Let $u^o_T(t)$ *be optimal control (23) on fixed time interval* $[0, T]$ *and suppose* $U \geq 1$*. Then:*

$$\forall\, \epsilon, \tilde{T} > 0,\ \exists\, T(\epsilon, \tilde{T}) > 0 :\ |u^o_{T(\epsilon,\tilde{T})}(t) - 1| \leq \epsilon,\ \forall\, t \in [0, \tilde{T}].$$

Optimal control of the one-dimensional reduction

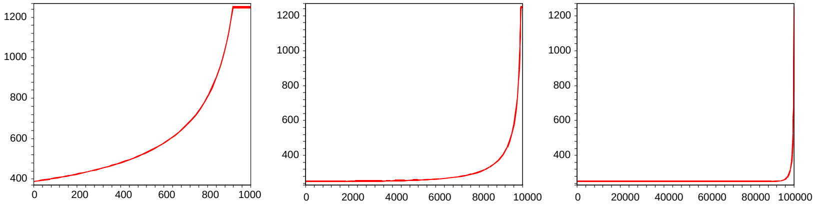

Figure: Optimal control of reduced system in μE $m^{-2}s^{-1}$; time in s.

More details (proof of reduction of approximation proposition, optimal control of one-dimensional reduction) in [Čelikovský, et al; TAC IEEE, 2010].

Conclusions

- Basics about PMP repeated.
- PSF dynamical model introduced and its properties described.
- Optimal control problem solved using one-dimensional reduction.
- Optimal production on increasing time intervals converges to the one generated by constant irradiance.
- Paradigm from biotechnological literature mathematically justificated.

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