Stability and optimization of the chemostat system including a linear coupling term between species[1]

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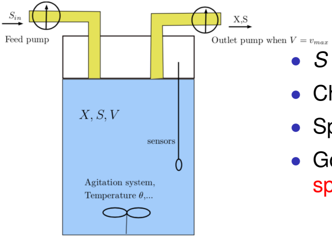
Outline

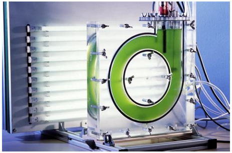
Plan

Modeling of a continuous bioreactor by the chemostat system



- S =resource ; X = consumer ; P = products
- Chemical reaction $S \rightarrow X + P$
- Speed pump : $u(t)$ = the control (for the input substrate $s_{in} > 0$)
- Goal : waste water treatment / selection / optimal production of species,...

$\Rightarrow$ bioenergy



Modeling of a bioreactor as an integro-differential system

- Consider a chemostat system with a phenotypical trait[2] and mutation:

$$\begin{cases} \partial_t x(t,\varphi) & = \mu(s(t),\varphi)x(t,\varphi) - u(t)x(t,\varphi) + \varepsilon\Delta_\varphi x(t,\varphi), \quad t>0 \quad \varphi \in \Omega \\ \frac{ds}{dt}(t) & = -\int_{\mathbb{R}_+^*} \mu(s(t),\varphi')x(t,\varphi)\mathrm{d}\varphi' + u(t)(s_{in} - s(t)), \quad t>0 \end{cases}$$

where $x =$ consumer ; $s =$ resource ; $\mu(0,\varphi) = 0$, $\forall \varphi \in \Omega$.

[2] Population dynamics model, see, *e.g.*, [Mirrahimi, Perthame, Wakano, '12]

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  where x = consumer ; s = resource ; $\mu(0,\varphi)=0$, $\forall\varphi\in\Omega$.
- Initial conditions + boundary conditions:

$$\begin{cases} s(0) &= s_0 \in (0,s_{in}), & \\ x(0,\varphi) &= x_0(\varphi)\geq 0, & \text{for all } \varphi\in\Omega, \\ \frac{\partial x}{\partial n}(t,\varphi) &= 0, & \text{for } t>0 \text{ and } \varphi\in\partial\Omega. \end{cases}$$

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- Objective : optimize w.r.t. $u \in L^\infty([0,T],[0,u_{max}])$

$$\max \int_0^T u(t) \left[\int_\Omega x(t,\varphi)\,\mathrm{d}\varphi \right] \mathrm{d}t$$

[2]Population dynamics model, see, *e.g.*, [Mirrahimi, Perthame, Wakano, '12]

Toward a discretization of the integro-differential system

- Existence /uniqueness of a solution for a given control function $t \mapsto u(t)$
- For a constant control $\bar{u}$, what is the asymptotical behavior of the system?
- Existence and characterization of an optimal control?

$\Rightarrow$ reduction / discretization in space

Reduction to a finite number of species

- Consider a chemostat system with a finite number of species:

$$\left| \begin{array}{lll} \dot{x}_i & = \mu_i(s)x_i - u(t)x_i + \varepsilon(Mx)_i, \; 1 \leq i \leq n, & x(0) = x_0 \in \mathbb{R}^n_+ \backslash \{0_{\mathbb{R}^n}\} \\ \dot{s} & = -\sum_{j=1}^{n} \frac{\mu_j(s)x_j}{Y_j} + u(t)(s_{in} - s), & s(0) = s^0 \in [0,1] \end{array} \right. \quad (1)$$

where $\varepsilon > 0$, $\mu_i : \mathbb{R}_+ \to \mathbb{R}_+$, $Y_j > 0$, $u \in L^\infty(\mathbb{R}_+, [0, u_{max}])$, and $M \in \mathbb{R}^{n \times n}$ is the symmetric quasi-positive irreducible matrix

$$M := \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & \cdots & 1 & -2 & 1 \\ 0 & \cdots & 0 & 1 & -1 \end{bmatrix} \Rightarrow \sum_{i=1}^{n} (Mx)_i = 0.$$

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- Objective function:

$$\max_{u(\cdot)\in[0,u_{max}]} \int_0^T \sum_{j=1}^{n} x_j(t)u(t)\,\mathrm{d}t$$

Plan

The dynamical system

$$\left| \begin{array}{lll} \dot{x} & = D(s)x - ux + \varepsilon Mx & x(0) = x_0 \in \mathbb{R}_+^n \backslash \{0\} \\ \dot{s} & = -\sum_{j=1}^{n} \mu_j(s) x_j + u(1-s) & s(0) \in [0,1] \end{array} \right. \quad (2)$$

- Kinetics : $\mu_i(s) := \frac{\bar{\mu}_i s}{k_i + s}$, $s \geq 0$ (Monod's kinetics)
- $D(s) := \mathrm{diag}(\mu_1(s), ..., \mu_n(s))$
- Parameters : $\varepsilon > 0$ and $u \in [0, +\infty)$.
- $Y_j = 1$ for $1 \leq j \leq n$ and $s_{in} = 1$.

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Some basic remarks:

- When $\varepsilon = 0$, we recover the usual chemostat system.
- Mass conservation : $m := \sum_{j=1}^n x_j + s$ is such that $\dot{m} = u(1-m) \Rightarrow m(t) \to 1$ as $t \to +\infty$ (provided that $u > 0$).

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- Mass conservation : $m := \sum_{j=1}^{n} x_j + s$ is such that $\dot{m} = u(1-m) \Rightarrow m(t) \to 1$ as $t \to +\infty$ (provided that $u > 0$).
- The fact that $m(t) \to 1$ is crucial ; it may fail to hold for a more general matrix M and if $Y_j \neq 1$

Local stability after regular perturbation

Define $u_c(\varepsilon) := \lambda(D(1) + \varepsilon M)$ where $\lambda(\cdot)$ denotes the Perron root.

Proposition (B., Cazenave-Lacroutz, Coville,'22)

- *For all* $(\varepsilon, u) \in \mathbb{R}_+^* \times (0, u_c(\varepsilon))$, (2) *has a unique LAS equilibrium* $E_{\varepsilon,u} \in \mathcal{D} := \mathbb{R}_+^n \backslash \{0\} \times [0,1]$ *called coexistence steady-state.*
- *In addition,* $E_{\varepsilon,u} = (x^{\varepsilon,u}, s^{\varepsilon,u})$ *with* $x_i^{\varepsilon,u} > 0$ *for every* $1 \leq i \leq n$ *where* $E_{\varepsilon,u} = (x^{\varepsilon,u}, s^{\varepsilon,u})$.
- *When* $\varepsilon \downarrow 0$, *one has* $E_{\varepsilon,u} = E_{i_0} + \varepsilon(\alpha, \beta) + o(\varepsilon)$ *where* $\alpha \in \mathbb{R}^n$ *is such that* $\alpha_i = 0$ *for* $i \notin \{i_0 - 1, i_0, i_0 + 1\}$ *and* $\beta < 0$.

When $\varepsilon = 0$, the system has $n + 1$ equilibria

$$\begin{array}{ll} E_{wo} & := (0, ..., 0, 1), \\ E_1 & := (1 - \mu_1^{-1}(u), 0, ..., 0, \mu_1^{-1}(u)), \\ \vdots & \vdots \\ E_{i_0} & := (0, .., 1 - \mu_{i_0}^{-1}(u), .., 0, \mu_{i_0}^{-1}(u)), \\ \vdots & \vdots \end{array}$$

and one GAS steady-state point E_{i_0} (competitive exclusion principle).

Global stability

- For $\varepsilon > 0$, GAS is a difficult (open) question!
- Counter-example : the system $\dot{x} = x\left(-\frac{1}{1+x^2} + \varepsilon\right)$ for which 0 is GAS for $\varepsilon = 0$ and LAS for every $\varepsilon \in [0,1)$. But 0 is never GAS for every $\varepsilon \in (0,1)$!
- In [De Leenheer et al.,'10], GAS is obtained provided that $Y_i \simeq 1$ and $\mu_i \simeq \mu_1$, $1 \leq i \leq n$

Theorem (B., Cazenave-Lacroutz, Coville,'22)

For all $\varepsilon > 0$, there is $u_s(\varepsilon) \in (0, u_c(\varepsilon)]$ s.t. for every $u \in (0, u_s(\varepsilon))$, $E^{\varepsilon,u}$ is GAS in $\mathcal{D}$.

- our initial objective was to address this question when $\varepsilon \downarrow 0$ (the question remains).
- the proof requires to derive persistence results about species.

H.L. Smith, P. Waltman, *Perturbation of a globally stable steady state*, Proc. Amer. Math. Soc., vol. 127, 2, pp. 447–453, 1999.

Plan

The optimal control problem

$$\left| \begin{array}{ll} \dot{x} & = D(s)x - u(t)x + \varepsilon Mx, \quad x(0) = x_0 \in \mathbb{R}_+^n \backslash \{0_{\mathbb{R}^n}\} \\ \dot{s} & = -\sum_{j=1}^{n} \mu_j(s)x_j + u(t)(1-s), \quad s(0) = s^0 \in [0,1] \end{array} \right. \tag{3}$$

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Given $T > 0$, the OCP reads as follows:

$$\boxed{\max_{u(\cdot)} \int_0^T u(t) \sum_{j=1}^{n} x_j(t)\, \mathrm{d}t}$$

- To simplify, we suppose that initial conditions are such that $\sum_{j=1}^{n} x_j^0 \leq 1$ and $s^0 + \sum_{j=1}^{n} x_j^0 = 1$.

Pontryagin's Principle

- Hamiltonian : $H(x,\lambda,u) := \sum_{j=1}^n \lambda_j x_j \mu_j + \varepsilon M\lambda \cdot x + u \underbrace{\sum_{j=1}^n (1-\lambda_j)x_j}_{\text{switching function } \phi}$
- Covector : $\dot{\lambda} = -\nabla_x H$ and $\lambda(T) = 0 \Rightarrow \phi(T) > 0$ and $\lambda > 0$ in some interval $[T-\eta, T)$
- Control law (except on singular arcs):

$$\begin{array}{lll} \phi(t) > 0 & \Rightarrow & u(t) = u_{max}, \\ \phi(t) < 0 & \Rightarrow & u(t) = 0, \end{array}$$

- Derivative of the switching function : $\dot{\phi} = \sum_{j=1}^n \mu_j x_j - (\sum_{j=1}^n x_j)(\sum_{j=1}^n \lambda_j x_j \mu_j')$.
- Along a singular arc, Legendre-Clebsch's necessary condition $\ddot{\phi}_u \geq 0$ must be verified:

$$\ddot{\phi}_{|u} = 2\Big(\sum_{j=1}^n x_j\Big)\sum_{j=1}^n \mu_j' x_j - \Big(\sum_{j=1}^n x_j\Big)^2 \sum_{j=1}^n \lambda_j x_j \mu_j'' \geq 0. \qquad \text{(LC)}$$

Conclusions about an (open loop) optimal control

Proposition

Every optimal extremal (x, λ, u) *is such that there exists* $\eta > 0$ *such that* $u(t) = u_{max}$ *and* $\lambda_i(t) > 0$ *for every* $t \in [T - \eta, T]$ *and* $1 \leq i \leq n$.

Conjecture

For every initial condition, an optimal control u (in open loop) is of turnpike type

$$B_{\pm} - S - B_{+} \tag{4}$$

and Legendre-Clebsch's condition is satisfied in the case of Monod's kinetics.

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- Difficulties : H is affine w.r.t. u, so, it is unclear if the turnpike result applies in this framework.
- Since $n \geq 1$ is large, LC condition is hard to check theoretically.

Numerical simulations via bocop (with the full system)

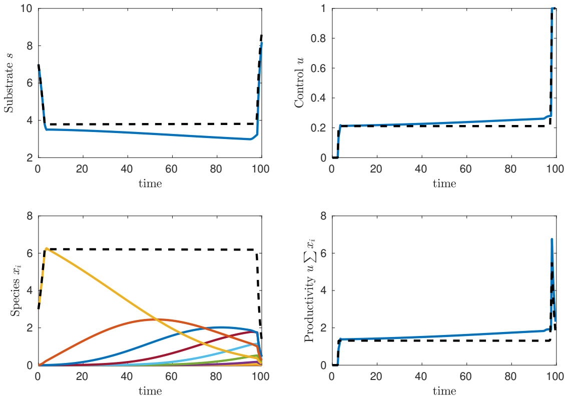


Figure: Solutions of the optimal control problem obtained with Bocop. The black dashed lines correspond to the case with one species without mutation. The color lines correspond to the same problem with mutation ($\varepsilon = 0.01$).

⇒ In any case, it is NOT evident to transfer a robust control law (like a feedback) to a practitionner.

Plan

The static OCP

- Goal : define robust control strategies approximating well the value function.
- Strategy:
  1. We compute the turnpike (static optimization problem) ;
  2. We construct (explicitly) feedback control laws (defining sub-optimal strategies)

$$\max_{(x,s,u)\in\mathcal{D}\times[0,u_{max}]} u\sum_{j=1}^{n} x_j \quad \text{s.t.} \quad \left| \begin{array}{ll} 0 & = D(s) - uI_n + \varepsilon M \\ 0 & = -\sum_{j=1}^{n} \mu_j(s)x_j + u(1-s) \end{array} \right.$$

where $\mathcal{D} := \mathbb{R}_+^n \backslash \{0_{\mathbb{R}^n}\} \times (0,1)$.

Static optimization

- For every $(\varepsilon, u) \in \mathbb{R}_+^* \times (0, u_c(\varepsilon))$, $(x^{\varepsilon,u}, s^{\varepsilon,u})$ is a steady-state of the system iff

$$\lambda(D(s) + \varepsilon M) = u \; ; \; \sum_{j=1}^{n} x_j + s = 1 \; ; \; (D(s) + \varepsilon M)x = ux. \tag{5}$$

Proposition

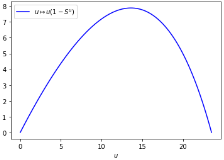
The static optimization problem

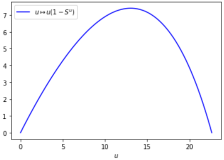
$$\max_{u \in [0, u_{max}]} u \sum_{j=1}^{n} x_j \quad \text{s.t. (5)}$$

is equivalent to

$$\max_{s \in (0,1)} (1 - s) \times \lambda(D(s) + \varepsilon M).$$

which has a solution $s_\varepsilon^\star \in (0, 1)$ (and a corresponding $u_\varepsilon^\star$ for the first problem).





- We expect the solution to be unique whenever the kinetics is of Monod type.

Definition of feedback control laws

Taking $u = u(x, s)$ yields

$$\dot{s} = -\sum_{j=1}^{n} \mu_j(s)x_j + u(x, s)(1 - s)$$

Fix $\sigma \in (0, 1)$. Plugging $u(x, s) = g_\sigma(x)$ with $g_\sigma(x) := \frac{1}{1-\sigma} \sum_{j=1}^{n} \mu_j(\sigma)x_j$ yields

$$\left| \begin{array}{ll} \dot{s} & = -\sum_{j=1}^{n} \mu_j(s)x_j + \varphi_\sigma(x)(1 - s), \\ s(t_0) & = \sigma \end{array} \right. \quad \Rightarrow s(t) = \sigma, \ \forall t \geq t_0.$$

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Proposition (B., Coville, Mairet, '22)

The closed-loop system (3) *with the feedback control* $g_\sigma(x) = \frac{1}{1-\sigma} \sum_{j=1}^{n} \mu_j(\sigma)x_j$ *or* $h_\sigma(s, x) := \frac{1}{1-\sigma} \sum_{j=1}^{n} \mu_j(s)x_j$ *is GAS in* $\mathcal{D}$ *around* $(\sigma, x^{\varepsilon,u})$ *where* $u := \lambda(D(\sigma) + \varepsilon M)$.

- the proof relies on an explicit integration of a Lotka-Volterra skew-symmetric type system

$$\dot{x}_i = \sum_{j} a_{i,j}x_i x_j, \quad 1 \leq i \leq n$$

after using the theory of asymptotically autonomous systems.

Optimal versus sub-optimal controls

Remind that the OCP reads as follows:

$$\max_{u(\cdot)\in\mathcal{U}} J_T(u) := \int_0^T u(t) \sum_{j=1}^n x_j(t)\,\mathrm{d}t \quad \text{s.t.}$$

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- Strategy 1 : **Optimal solution** (bocop) ;
- Strategy 2 : **Constant control** : apply $u = u_\varepsilon^\star$ after solving the static OCP ;
- Strategy 3 : **Feedback controlled** apply $u = \varphi_\sigma$ or $u = \psi_\sigma(s,x)$ with $\sigma = s_\varepsilon^\star$.

Optimal versus sub-optimal controls

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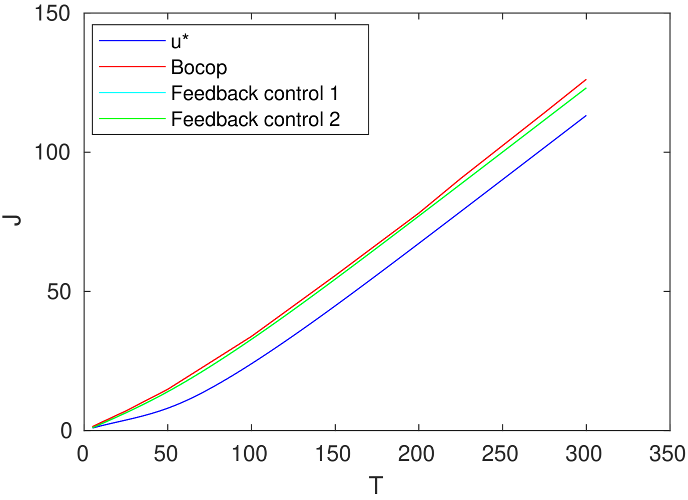
- Strategy 1 : **Optimal solution** (bocop) ;
- Strategy 2 : **Constant control** : apply $u = u^\star_\varepsilon$ after solving the static OCP ;
- Strategy 3 : **Feedback controlled** apply $u = \varphi_\sigma$ or $u = \psi_\sigma(s,x)$ with $\sigma = s^\star_\varepsilon$.

Observe that Strategy 2 and 3 do not depend on the initial condition.

Numerical gap between optimal and sub-optimal controls



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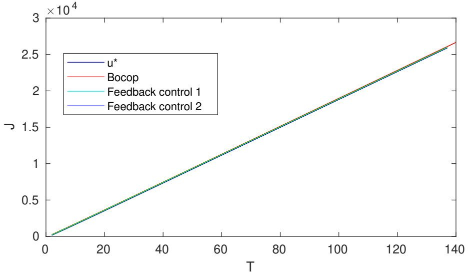

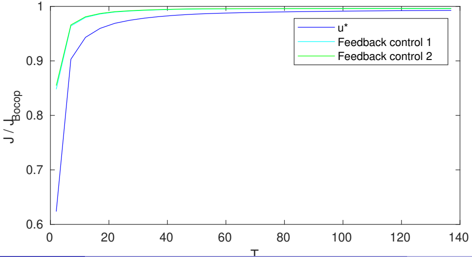

Conclusion and perspectives

Conclusions:

- Two main contributions :
  - LAS and GAS (provided that u is small enough) of the chemostat system with mutation
  - GAS stability for the closed-loop system with $u = g_\sigma(x, s)$ or $u = h_\sigma(x, s)$
- The PMP provides qualitative properties of optimal paths (in open loop) ;
- Sub-optimal feedback controls are of great interest in presence of uncertainties. From a practical point of view, h_σ corresponds to biogas production (can be measured) ;
- The gap between the value function and the cost of sub-optimal controls (defined by φ_σ and ψ_σ) tends to be very small as $T \to +\infty$.

Perspectives:

- Generalize to the PDE model (existence of a solution / convergence, stabilization of the integro-differential system)
- Prove the GAS stability (using Lyapunov functions or other methods)
- Generalize the study (dynamical system properties ; OCP) to Haldane kinetics and whenever the mutation factor is more general (and $Y_i \neq 1$).

References

Thank you for your attention

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