Optimal allocation of bacterial resources in a bioreactor

Introduction to optimal control problems

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Summary

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* Introduction to the problem
* Definition of the model
* Understanding optimal control theory
* The biomass maximisation case
* Calculation of Lie brackets
* Conclusion

» Introduction to the problem

The study of living micro-organisms

Bacteria's resource management and compound production in batch bioprocessing are explored using mathematical models, revealing insights at the biology-engineering crossroads.
How can one know how to maximize the needs of a bacteria for its optimal development ?

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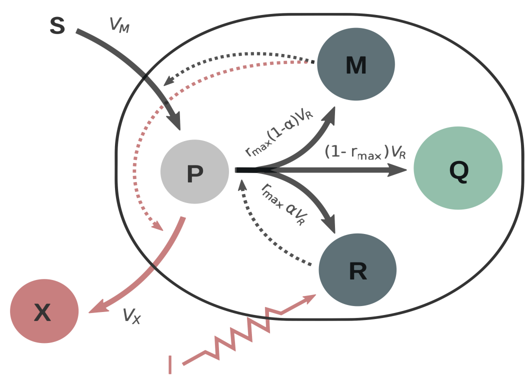
» Definition of the model



The self-replicator model

» Definition of the model

- Initial mass of **substrate** S
- Transformed into **precursors metabolites** P
- P produces M, Q and R which catalyze other productions
- Creation of X, **metabolites of interest**

» Definition of the model

Dynamical system

$$
\begin{cases}
\dot{S} &= -V_M \\
\dot{P} &= V_M - V_X - V_R \\
\dot{R} &= r_{max} u V_r \\
\dot{M} &= r_{max}(1-u)V_R \\
\dot{Q} &= (1-r_{max})V_R \\
\dot{X} &= V_X
\end{cases}
\tag{SRM-D}
$$

Summary

» Understanding optimal control theory

Optimal control theory deals with objects that are to be **controlled** meaning that they depend on external factors. Example for a plant growth :

* Temperature
* Lightning
* Water
* and much more ...

These are some of the many "controls" that one can try to adjust to maximize the plant growth.

» Understanding optimal control theory

Mathematical explanation

Let's say we want to maximize a plant's height.
This can be modeled as follows : Let $u \in \mathbb{R}$, $x \in \mathbb{R}^2$, $t \in [t_0, t_f]$, $x(t_0) = [h_0, s_0]$, h_0 being the height of the plant at time $= 0$ and s_0 the thickness of the stem at time $= 0$.
An example of the control u could be for example the light intensity variation over time, or the variation of temperature over time.

$$\begin{cases} \dot{x}(t) = F_0(x(t)) + u(t) \cdot F_1(x(t)) \\ h(t_f) \longrightarrow max \end{cases}$$

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» The biomass maximisation case

Finite-time problem

$$\begin{cases} \dot{s} = -w_M(s)(1-r)\mathcal{V} \\ \dot{p} = w_M(s)(1-r) - w_R(p)(1+p)r \\ \dot{r} = (u-r)w_R(p)r \\ \dot{\mathcal{V}} = w_R(p)r\mathcal{V} \end{cases} \tag{WTB-M}$$

» The biomass maximisation case

Finite-time problem

The numerical simulations of (WTB-M) were already done for a infinite-time problem. As a result, we solved the OCP problem for a finite-time horizon.

» The biomass maximisation case

Definition of $(\boldsymbol{BM-OCP})$

The problem in a finite-time case is modeled as follows

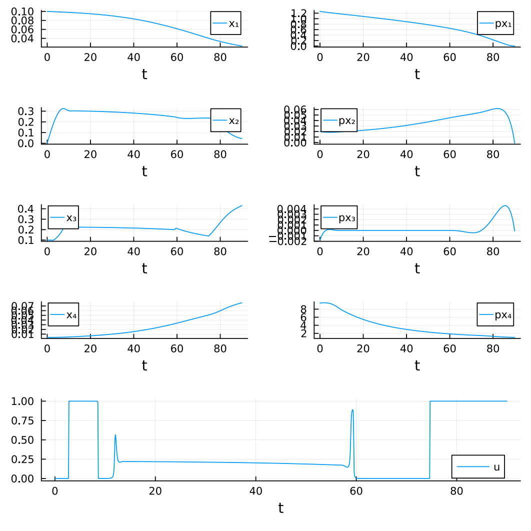
$$\begin{cases} \mathcal{V}(t_f) \longrightarrow max \\ \text{using the dynamics of (WTB-M)} \\ \text{using initial conditions (IC)} \\ u \in \mathcal{U} \end{cases} \qquad \text{(BM-OCP)}$$

With (IC) being

$$\begin{aligned} s(0) = s_0 > 0, p(0) = p_0 > 0, x(0) = 0, r(0) = r_0 \in (0,1), \\ \mathcal{V}(0) = \mathcal{V}_0 > 0 \end{aligned} \qquad \text{(IC)}$$

» The biomass maximisation case

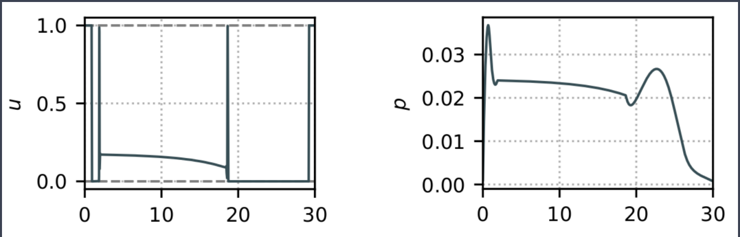
Results of the numerical simulations



Numerical simulations of (BM-OCP)

» The biomass maximisation case

Results of the numerical simulations



Numerical simulations of (BM-OCP)

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» Calculation of Lie brackets

Proposition to be proved

Proposition 4.4

If the *Lie* bracket F_{101} belongs to the span of F_1 and F_{01}, then singular extremals must be of (local) order at least two.

Since our problem is modeled as follows

$$\varphi(x) = F_0(x) + u \cdot F_1(x)$$

with $x = (s\ p\ r\ \mathcal{V})^t$ with respect to (WTB-M)
our goal was to compute the *Lie* brackets $F_{01} = [F_0, F_1]$ and $F_{101} = [F_1, F_{01}]$ and to make sure that

$$rank(F_1(\varphi), F_{01}(\varphi)) = rank(F_1(\varphi), F_{01}(\varphi), F_{101}(\varphi))$$

A *Lie* bracket is defined for vector fields as $[X, Y] = Y'X - X'Y$

» Introduction to Lie brackets

The calculation of *Lie* brackets are involving determinants of 4×4 matrices which can be quite tricky to do by hand. Hence, we decided to use symbolic calculation with `Julia`

Summary

» Conclusion

This project was for us a glance at what research really is :

* hand-calculations are not always possible
* Julia is great for mathematicians
* we liked working in english as it helped us getting better