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Optimization of the separation of two species in a chemostat

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Abstract

In this work, we study a two species chemostat model with one limiting substrate, and our aim is to optimize the selection of the species of interest. More precisely, the objective is to find an optimal feeding strategy in order to reach in minimal time a target where the concentration of the first species is significantly larger than the concentration of the other one. Thanks to Pontryagin maximum principle, we introduce a singular feeding strategy which allows to reach the target, and we prove that the feedback control provided by this strategy is optimal whenever initial conditions are chosen in the invariant attractive manifold of the system. The optimal synthesis of the problem in presence of more than one singular arc and for initial conditions outside this set is also investigated.

Key words: Chemostat; Optimal control; Pontryagin maximum principle.

1 Introduction

Selection of species has been widely used in agriculture and biotechnology in order to improve productivity. For microorganisms, the selection process can be based on genetic tools. Another way to proceed is to drive the competition between species in a chemostat. In this case, a control strategy should be defined adequately in order to select species according to a given criteria (see e.g. [10,11]).

Here, we consider a two species chemostat limited by one substrate with Monod-like growth functions (see [13]). The following property known as the competitive exclusion principle is standard in the theory of chemostat (see [13]): given a constant dilution rate, the species which can grow at a rate equal to the dilution with the smallest substrate concentration survives whereas the other one disappears as time goes to infinity. This approach can be used in order to select asymptotically one of the two species provided that the dilution rate is adequately chosen.

In this paper, we propose an alternative approach based on optimal control theory in order to reach in finite time a certain target where the concentration of a given species is significantly larger than the other one. More precisely, our aim is to find an optimal feeding strategy in order to steer the system to this target in minimal time.

To characterize optimal trajectories, we proceed as follows. We first assume that initial conditions are in the invariant attractive set of the system (see [13]), so that it can be put into a two-dimensional affine controlled system with a single input. In our setting, the target is defined by a hyperplane and is not a target point, and one can see that there exists a subset of the set of initial conditions where the two vector fields defining the system are collinear. It follows that it is not possible to use the clock form to conclude rapidly on the optimal feeding strategy (see e.g. [2,4,12]). Thanks to Pontryagin maximum principle and cooperatively properties of the adjoint system, we overcome this difficulty, and we show that it is not optimal for a trajectory to have a switching point before reaching either the target or the singular arc. This leads to a complete description of optimal trajectories in the case where initial conditions are taken in this set. Theorem 2 is our main result and states that the optimal strategy is singular. In other words, the optimal feedback control corresponds to a most rapid approach (see [6]) to a singular arc (if it is reached).

The study of optimal controls for initial conditions outside the invariant set is more difficult as the system cannot be reduced to a two-dimensional one. Nevertheless,
we can prove that a singular arc which intersects the target is characterized in the same way as in the two-dimensional case. This is a first step in the proof of an extension of Theorem 2 in this setting. Numerical solutions of the problem via a direct method (see [3]) confirm this result.

The paper is organized as follows. The second section is devoted to the statement of the optimal control problem. In the third section, we apply Pontryagin maximum principle in order to derive necessary conditions on optimal trajectories. In the fourth section, we introduce the singular arc strategy, and we prove that it is optimal for reaching the target (Theorem 2). We also investigate the selection of the second species (Theorem 3), and we study the case where initial conditions are taken outside the invariant set. The last section discusses the problem in presence of more than one singular arc (which may happen with Haldane-like growth functions).

2 Statement of the problem

A chemostat model with one limited resource, two species, and adimensional yield coefficients can be modeled as follows (see [13]):

$$\begin{align*}
\dot{x}_1 &= \mu_1(s) - u_x_1, \\
\dot{x}_2 &= \mu_2(s) - u_x_2, \\
\dot{s} &= -\mu_1(s)x_1 - \mu_2(s)x_2 + u(s_\text{in} - s).
\end{align*}$$

(1)

Here, $x_1$ (resp. $x_2$) is the concentration of the first (resp. second) species in the reactor, $s$ is the concentration of substrate, $s_\text{in}$ is the input substrate concentration, $u$ is the dilution rate, and $\mu_i$ are the growth functions of the two species. In the following, we suppose that the specific growth rates of both species $\mu_i$, $i = 1, 2$ are nonnegative increasing $C^1$ functions with $\mu_i(0) = 0$. We will also impose the following assumption on the growth functions.

**Hypothesis 1** The growth functions of the two species fulfill the following conditions:

- there exists a unique $\hat{s} > 0$ such that $\mu_1(\hat{s}) = \mu_2(\hat{s})$
- the function $s \mapsto \mu_1(s) - \mu_2(s)$ is increasing on $(0, \hat{s})$, and decreasing on $(\hat{s}, +\infty)$, with $\hat{s} < \hat{s}$.

For example, Hypothesis 1 is fulfilled for two growth rates of type Monod (see Fig 1):

$$\mu_1(s) := \frac{\overline{\mu}_1 s}{k_1 + s}, \quad \mu_2(s) := \frac{\overline{\mu}_2 s}{k_2 + s},$$

(2)

with $\overline{\mu}_1k_2 > \overline{\mu}_2k_1$, $\overline{\mu}_1 < \overline{\mu}_2$, implying $k_2 > k_1$, $\mu_1(0) > \mu_2(0)$, and:

$$\hat{s} = \frac{\overline{\mu}_1k_2 - \overline{\mu}_2k_1}{\overline{\mu}_2 - \overline{\mu}_1}, \quad \hat{s} := \frac{k_2}{\sqrt{\overline{\mu}_1k_1} - k_1\sqrt{\overline{\mu}_2k_2}} - \sqrt{\overline{\mu}_2k_2} - \sqrt{\overline{\mu}_1k_1}.$$

The competitive exclusion principle in presence of two species can be stated as follows (see [13]).

**Theorem 1** Let us consider a constant dilution rate $u < \max(\mu_1(s_\text{in}), \mu_2(s_\text{in}))$ and assume that hypothesis 1 holds. Then, for any initial condition $x_i(0) > 0$, $i = 1, 2$, system (1) satisfies the following property.

(i) If $u < \mu_1(\hat{s})$, and $\lambda_1$ is such that $\mu_1(\lambda_1) = u$, then:

$$\lim_{t \to +\infty} s(t) = \lambda_1, \quad \lim_{t \to +\infty} x_1(t) = s_\text{in} - \lambda_1, \quad \lim_{t \to +\infty} x_2(t) = 0.$$

(ii) If $u > \mu_1(\hat{s})$, and $\lambda_2$ is such that $\mu_2(\lambda_2) = u$, then:

$$\lim_{t \to +\infty} s(t) = \lambda_2, \quad \lim_{t \to +\infty} x_2(t) = s_\text{in} - \lambda_2, \quad \lim_{t \to +\infty} x_1(t) = 0.$$

The concentrations $\lambda_i$ are called break-even concentrations, see [13]. If $u = \mu(\hat{s})$, the coexistence of the two species is possible (in practice it is difficult to choose exactly a dilution rate $u$ such that $u = \mu(\hat{s})$). In the previous theorem, choosing an adequate dilution rate allows to select one of the two species, however the convergence to the equilibrium is in infinite horizon. In this work, our aim is to find an adequate feeding strategy in order to reach in finite time a target set where the concentration of one of the two species is significantly larger than the other one.

In order to simplify the system, we will make the following requirements. Let $M := x_1 + x_2 + s$ denotes the total mass of the system, which satisfies:

$$M = u(s_\text{in} - M).$$

(3)

From (3), it is standard that the set

$$F := \{(x_1, x_2, s) \in \mathbb{R}_+^* \times \mathbb{R}_+^* \times \mathbb{R}_+^* \mid x_1 + x_2 + s = s_\text{in}\},$$

is invariant and attractive for system (1), see [13]. From now on, we assume that initial conditions are in the set $F$, so that the triple $(x_1, x_2, s)$ satisfies:

$$x_1 + x_2 + s = s_\text{in}.$$  

(4)

System (1) becomes a two-dimensional affine system with one input $u$:

$$\begin{align*}
\dot{x}_1 &= [\mu_1(s) - u]x_1, \\
\dot{x}_2 &= [\mu_2(s) - u]x_2,
\end{align*}$$

(5)

where $s = s_\text{in} - x_1 - x_2$. The set of admissible controls for (5) is given by:

$$U := \{u : [0, +\infty) \to [0, u_{\text{max}}] \mid \text{meas.}\},$$

2
where $u_{\text{max}}$ denotes the maximum dilution rate. As $s$ is positive, initial conditions are in the set

$$ E := \{(x_1, x_2) \in \mathbb{R}^*_+ \times \mathbb{R}^*_+ \mid x_1 + x_2 < s_i\}, $$

which is invariant with respect to (5). We are now in position to state the optimal control problem. Let $\varepsilon > 0$ a small parameter, and let us consider a target $T$ defined as follows. In order to select the first species, the target $T_1$ is:

$$ T_1 := \{(x_1, x_2) \in E \mid x_2 \leq \varepsilon x_1\}, $$

whereas if the objective consists in selecting the second one, the target is:

$$ T_2 := \{(x_1, x_2) \in E \mid \varepsilon x_2 \geq x_1\}. $$

The optimal control problem reads as follows. Given $x_0 := (x_0^1, x_0^2) \in E$, our aim is to find an admissible control $u \in U$ steering the solution $x(\cdot)$ of (5) from $x_0$ to the target in minimal time:

$$ \inf_{u \in U} t(u) \text{ s.t. } x(t(u)) \in T, $$

where $T$ is either $T_1$ or $T_2$, and $t(u)$ is the first entry time in the target.

Without any loss of generality, we may assume that $u_{\text{max}} = 1$. The next assumption is standard and means that the maximum value of the input flow rate can be larger than the growth of microorganisms (see e.g. [1,8]):

**Hypothesis 2** The growth function $\mu_1$ and $\mu_2$ satisfy:

$$ \max_{s \in [0, s_i]} (\mu_1(s), \mu_2(s)) < 1. $$

The next assumption means that the input substrate concentration has been chosen large enough such that both species can win the competition.

**Hypothesis 3** The input substrate concentration $s_i$ satisfies:

$$ s_i > \hat{s}. $$

**Remark 1** (i) For any initial condition $x^0 \in E$, there exists a control $u \in U$ steering (5) to the target $T_i$, $i = 1, 2$. Indeed, one can apply Theorem 1 with a constant control $u$ such that either $u < \mu_1(\hat{s})$ or $u > \mu_1(\hat{s})$ in order to select the first species or the second one.

(ii) By the previous remark, the compactness of the control set, and the linearity of (5) with respect to $u$, one can apply Filippov’s Theorem (see e.g. [9]) in order to prove the existence of an optimal control for (6).

We now introduce subsets of $E$ that will play a major role in the optimal synthesis of the problem (see section 4). Let us write (5) as a two-dimensional affine system with a drift:

$$ \dot{x} = f(x) + ug(x), $$

where $x := (x_1, x_2)$ and $f, g : \mathbb{R}^+ \times \mathbb{R}^+ \to \mathbb{R}^2$ are the two vector fields of class $C^\infty$ given by

$$ f(x) := \left(\begin{array}{c} \mu_1(s)x_1 \\ \mu_2(s)x_2 \end{array}\right), \quad g(x) := \left(\begin{array}{c} -x_1 \\ -x_2 \end{array}\right), $$

with $s = s_i - x_1 - x_2$. We define $\gamma$ as the determinant of $f$ and $g$:

$$ \gamma(x) := \det(f(x), g(x)) = x_1x_2[\mu_2(s) - \mu_1(s)], $$

so that $\gamma(x) = 0$ if and only if $s = \hat{s}$, that is $x$ belongs to the set:

$$ \Delta_0 := \{(x_1, x_2) \in E \mid x_1 + x_2 = \hat{x}\}, $$

where $\hat{x} := s_i - \hat{s}$. Let $[f, g]$ the Lie bracket of $f$ and $g$ (see e.g. [4]). We define a subset $\Delta_{SA} \subset E$ as the set of points where $\det(g(x), [f, g](x)) = 0$. This set is called singular arc and plays a major role in the optimal synthesis. In our setting, we have:

$$ \Delta_{SA} := \{(x_1, x_2) \in E \mid x_1 + x_2 = \overline{\tau}\}, $$

where $\overline{\tau} := s_i - \hat{s} > \hat{x}$.

**Remark 2** Notice that it is not possible to apply the clock form argument globally in this framework (see [4,12]). First, the target is not an isolated point, hence optimal trajectories may have different terminal points. Moreover, if we consider an initial point $x_0 \in \{\gamma > 0\}$ and a terminal point $x_1 \in \{\gamma < 0\}$, trajectories steering $x_0$ to $x_1$ will intersect the set $\Delta_0$.

<table>
<thead>
<tr>
<th>$k_1$</th>
<th>$\overline{n}_1$</th>
<th>$k_2$</th>
<th>$\overline{n}_2$</th>
<th>$s_i$</th>
<th>$\varepsilon$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5</td>
<td>8</td>
<td>1</td>
<td>10</td>
<td>0.1</td>
</tr>
</tbody>
</table>

Table 1
Values of the parameters (arbitrary units) in Fig. 1 and 2 with $\mu_1$ and $\mu_2$ given by (2).

![Fig. 1](image-url)

Left: plot of the growth functions $\mu_1$ (in blue) and $\mu_2$ (in green) satisfying Hypothesis 1. Right: plot of $s \mapsto \mu_1(s) - \mu_2(s)$. Parameters of the growth functions are given in Table 1 (arbitrary units).
3 Pontryagin maximum principle

In this part, we apply Pontryagin maximum principle (PMP) on the minimum time problem and we obtain necessary conditions on optimal trajectories.

Let \( H = H(x_1, x_2, \lambda_1, \lambda_2, \lambda_0, u) \) the Hamiltonian of the system defined by:

\[
H := \lambda_1 \mu_1(s)x_1 + \lambda_2 \mu_2(s)x_2 + \lambda_0 + u[-\lambda_1 x_1 - \lambda_2 x_2].
\]

Let \( u \) an optimal control, and \( x(\cdot) \) the associated trajectory. There exists \( t_f > 0 \), an absolutely continuous map \( \lambda : [0, t_f] \rightarrow \mathbb{R}^2 \), and \( \lambda_0 \leq 0 \) such that \( (\lambda(\cdot), \lambda_0) \neq 0 \), \( \lambda(\cdot) \) satisfies the adjoint equation \( \dot{\lambda} = -\frac{\partial H}{\partial x}(x(t), \lambda(t), \lambda_0, v) \), that is:

\[
\begin{align*}
\dot{\lambda}_1 &= \lambda_1 \mu'_1(s)x_1 - \mu_1(s) + \lambda_2 \mu'_2(s)x_2 + \lambda_1 u, \\
\dot{\lambda}_2 &= \lambda_2 \mu'_2(s)x_2 - \mu_2(s) + \lambda_1 \mu'_1(s)x_1 + \lambda_2 u,
\end{align*}
\]

and we have the maximization condition:

\[
u(t) \in \text{argmax}_{v \in [0, 1]} H(x(t), \lambda(t), \lambda_0, v), \text{ a.e. } t \in [0, t_f].
\]

Notice that the adjoint system is cooperative (i.e. it satisfies \( \frac{\partial H}{\partial \lambda_i} > 0 \) for \( i \neq j \)). This property is used in the next section. An extremal trajectory is a quadruplet \( (x(\cdot), \lambda(\cdot), \lambda_0, u(\cdot)) \) satisfying (5)-(8)-(9). From (9), we have that the control law is given by the sign of the switching function defined by:

\[
\phi := -\lambda_1 x_1 - \lambda_2 x_2.
\]

Hence, we have by (9):

\[
\begin{align*}
u &= 1 \iff \phi > 0, \\
u &= 0 \iff \phi < 0.
\end{align*}
\]

Whenever the control \( u \) is non-constant in any neighborhood of a time \( t_0 \in (0, t_f) \), we say that \( t_0 \) is a switching point. It follows that \( \phi \) is vanishing at time \( t_0 \). Whenever \( \phi \) is vanishing over a time interval \( I = [t_1, t_2] \), we say that the trajectory contains a singular arc. As the terminal time is not fixed, the Hamiltonian is zero along any extremal trajectory. Moreover, the transversality condition reads as follows (see [14]):

\[
\lambda(t_f) \in -N_T(x(t_f)),
\]

where \( N_T(x(t_f)) \) is the normal cone to \( T \) at the point \( x(t_f) \) (\( \langle \cdot, \cdot \rangle \) denotes the scalar product in \( \mathbb{R}^2 \)):

\[
N_T(x(t_f)) := \{ \xi \in \mathbb{R}^2 \mid \langle \xi, y - x(t_f) \rangle \leq 0, \forall y \in T \}.
\]

From the definition of \( T_1 \), (11) implies that \( \lambda(t_f) \) is parallel to the vector \( n := \frac{(e_1, -e_2)}{\| (e_1, -e_2) \|} \). By Pontryagin maximum principle, an optimal trajectory necessarily satisfies (11), and therefore we have \( \phi(t_f) = 0 \) (recall (10)).

**Lemma 3** Consider an optimal trajectory starting at some point \((x_1^0, x_2^0) \notin T \), and assume that the trajectory reaches the target at a substrate concentration \( s(t_f) \neq \hat{s} \). Then, we have \( \lambda_0 \neq 0 \).

**PROOF.** Assume that \( \lambda_0 = 0 \). At the terminal time, the transversality condition implies \( \phi(t_f) = 0 \). It follows that the adjoint vector at time \( t_f \) is orthogonal to \( g(x(t_f)) \). From \( H = 0 \), we deduce that \( \lambda(t_f) \) is also orthogonal to \( f(x(t_f)) \), hence we have \( \lambda(t_f) = 0 \) as \( f \) and \( g \) are linearly independent at \( x(t_f) \), which is a contradiction.

Next, we assume that \( \lambda_0 \neq 0 \), and without any loss of generality that \( \lambda_0 = -1 \). We will see in the next section that it is not optimal for a trajectory to reach the target at \( s = \hat{s} \). By conservation of the Hamiltonian along an extremal trajectory together with the free terminal time, we obtain:

\[
\lambda_1 \mu_1(s)x_1 + \lambda_2 \mu_2(s)x_2 - 1 + u[-\lambda_1 x_1 - \lambda_2 x_2] = 0.
\]

The next lemma gives the sign of the adjoint vector at a switching point.

**Lemma 4** Let \( t_0 \) be a switching point such that \( s(t_0) \neq \hat{s} \). Then, we have:

\[
\begin{align*}
\lambda_1(t_0) &= \frac{1}{x_2(t_0)[\mu_2(s(t_0)) - \mu_1(s(t_0))]}, \\
\lambda_2(t_0) &= \frac{1}{x_2(t_0)[\mu_2(s(t_0)) - \mu_1(s(t_0))]}. \\
\end{align*}
\]

**PROOF.** It is straightforward using (10) and (12).

We now analyze singular trajectories. By differentiating \( \phi \) with respect to \( t \), we get:

\[
\dot{\phi} = -[x_1 + x_2][\lambda_1 \mu'_1(s) + \lambda_2 \mu'_2(s)],
\]

and for future reference, we define \( \psi := \lambda_1 x_1 \mu'_1(s) + \lambda_2 x_2 \mu'_2(s) \). Let \([t_1, t_2]\) be a time interval where \( \phi(t) = 0 \), for all \( t \in [t_1, t_2] \). Then, we have \( \psi(t) = 0 \) for all \( t \in [t_1, t_2] \). This implies that \( s(t) = \overline{s} \) for all \( t \in [t_1, t_2] \) (otherwise, we would have \( \lambda_1 = \lambda_2 = 0 \) in contradiction with Pontryagin maximum principle). Hence, the singular arc is contained in the set \( \Delta_{SA} \). By (5), we can define a singular control \( u_{\overline{s}} \) by:

\[
u_{\overline{s}} := \frac{\mu_1(\overline{s})x_1 + \mu_2(\overline{s})x_2}{x_1 + x_2}.
\]
From the expression above and (7), the singular control \( u_{\pi} \) satisfies \( u_{\pi} \in [0, 1] \), hence the singular arc is always controllable. From (12), we obtain that \( \lambda \) is given by (13) with \( \bar{s} \) in place of \( s \). Therefore, we have \( \lambda_1 < 0 \) and \( \lambda_2 > 0 \) along a singular arc. Moreover, (5) with \( u = u_{\pi} \) becomes:

\[
\begin{align*}
\dot{x}_1 &= \frac{x_1 x_2}{x_1 + x_2} [\mu_1(\bar{s}) - \mu_2(\bar{s})], \\
\dot{x}_2 &= \frac{x_1 x_2}{x_1 + x_2} [\mu_2(\bar{s}) - \mu_1(\bar{s})],
\end{align*}
\]

so that the singular trajectory satisfies \( \dot{x}_1 > 0 \) and \( \dot{x}_2 < 0 \) (recall Hypothesis 1). By definition of the target, we have that any singular trajectory reaching the target satisfies the transversality condition.

4 Optimal synthesis

The main purpose of this section is to characterize the optimal feeding strategy in order to reach \( T_1 \) (see Theorem 2) and \( T_2 \) (see Theorem 3). We also address the case where initial conditions are outside the invariant set.

4.1 Partition of the domain

The next definition introduces the singular arc strategy. Hereafter, \( T_1^c \) denotes the complementary of \( T_1 \) in \( E \).

**Definition 1** For \((x_1^0, x_2^0) \in T_1^c \), the singular arc strategy \( S_A \) is a mapping of the feedback control law given by:

\[
\begin{align*}
 u &= 1 \iff s_0 < \bar{s}, \\
 u &= 0 \iff s_0 > \bar{s}, \\
 u &= u_{\pi} \iff s_0 = \bar{s},
\end{align*}
\]

where \( s_0 := s_{in} - x_1^0 - x_2^0 \) and \( u_{\pi} \) is given by (15).

This strategy steers any initial condition \((x_1^0, x_2^0) \in E \) to the target \( T_1 \) provided \( \mu_1(\bar{s}) > \mu_2(\bar{s}) \). Indeed, if \( s_0 < \bar{s} \), we have that \( s := s_{in} - x_1 - x_2 \) satisfies \( \dot{s} > 0 \) with \( u = 1 \), and either the trajectory reaches the target, or it reaches the singular arc \( \Delta_s \). In the latter case, the target is reached by choosing \( u = u_{\pi} \) (recall (16)). Whenever \( s_0 > \bar{s} \), the trajectory reaches either the target or the singular arc, and the same conclusion follows.

The next variable change will be useful in the following. Let \( \mu \) denotes the proportion of the first species in the chemostat:

\[
p := \frac{x_1}{x_1 + x_2}.
\]

We easily obtain \( x_1 = p(s_{in} - s) \) and \( x_2 = (1 - p)(s_{in} - s) \), so that (5) is equivalent to the system:

\[
\begin{align*}
\dot{p} &= p(1 - p)[\mu_1(s) - \mu_2(s)], \\
\dot{s} &= -p \mu_1(s) - (1 - p) \mu_2(s) + u(s_{in} - s).
\end{align*}
\]

Notice that the first equation of (19) does not depend on the control variable \( u \). Moreover, we have \( p(0) \in (0, 1) \) so that \( p(t) \in (0, 1) \) for all \( t \) by Cauchy-Lipschitz Theorem. Also, we have \( \dot{p} > 0 \) iff \( s < \bar{s} \) and \( \dot{p} = 0 \) iff \( s = \bar{s} \). Recall from (7) that we have \( \dot{s} > 0 \) in (19) whenever \( u = 1 \). Next, consider the intersection point between \( \Delta_0 \) and \( T_1 \) (which is of coordinates \((x_1^*, x_2^*) \)) and let us define \( x^\dagger := (x_1^*, x_2^*) \) as the unique solution of (5) backward in time with \( u = 1 \), and starting at the point \((x_1^*, x_2^*) \). Let \((y_1^*, y_2^*) \) its intersection with the singular arc \( \Delta_{S_A} \) (recall the monotonicity property of (5) with \( u = 1 \)). As \( t \mapsto x^\dagger(t) \) is one-to-one, there exists a mapping \( F : [x_1^*, y_1^*] \mapsto \mathbb{R} \) which is local Lipschitz, and such that the graph of \( F \) coincides with \( x^\dagger \) until \((y_1^*, y_2^*) \). To prove the main result, we consider the following partition of \( T_1^c \) into the four subsets \( A, B, C, \) and \( D \) defined by:

\[
\begin{align*}
 A &:= \{(x_1, x_2) \in T_1^c \mid x_2 > F(x_1) \} \quad \text{in which} \quad F(x_1) = x_1, \\
 B &:= \{(x_1, x_2) \in T_1^c \mid x_2 \leq F(x_1) \} \\
 C &:= \{(x_1, x_2) \in T_1^c \mid x_1 + x_2 \leq 2\bar{s} \}, \\
 D &:= \{(x_1, x_2) \in T_1^c \mid x_1 + x_2 > 2\bar{s} \}.
\end{align*}
\]

**Remark 5** A trajectory with a constant control \( u = 1 \) starting in the set \( B \) will reach the target \( T_1 \) whereas if it starts in \( A \cup C \), then it will not reach \( T_1 \).

4.2 Optimal synthesis in the case of \( T_1 \)

The two next lemmas are based on the cooperativity property of the adjoint system and are fundamental in order to prove Theorem 2.

**Lemma 6** Let us consider an optimal trajectory starting from \((x_1^0, x_2^0) \in A \cup B \cup C \), and suppose \( \phi(0) < 0 \).

(i) Then, we have \( \lambda_1(t) > 0 \) and \( \lambda_2(t) < 0 \).

(ii) If \([0, t_0) \) is the maximal time interval where \( \phi < 0 \), then \( \lambda_1(t) > 0 \) and \( \lambda_2(t) < 0 \) for any \( t \in [0, t_0) \).

**PROOF.** For convenience, we write \((\hat{\lambda}_1, \hat{\lambda}_2) := (\lambda_1, \lambda_2)\). At time zero, there are three possible cases: the initial adjoint vector either satisfies \( \hat{\lambda}_1 > 0 \) and \( \hat{\lambda}_2 > 0 \) (case a), or \( \hat{\lambda}_1 < 0 \) and \( \hat{\lambda}_2 > 0 \) (case b), or \( \hat{\lambda}_1 > 0 \) and \( \hat{\lambda}_2 < 0 \) (case c). The transversality condition implies the existence of a time \( t' > 0 \) such that \( \phi(t') = 0 \). Notice also from (8) that both \( \hat{\lambda}_1 \) and \( \hat{\lambda}_2 \) cannot vanish at a same instant.

Case a. Let \( t_0 > 0 \) the first time where \( \phi(t_0) = 0 \). Necessarily, there exists \( 0 < t_1 < t_0 \) such that \( \hat{\lambda}_1(t_1) = 0 \) or \( \hat{\lambda}_2(t_1) = 0 \) (otherwise \( \phi \) would not vanish at time \( t_0 \)). If \( t_1 \) is such that \( \hat{\lambda}_1(t_1) = 0 \) and \( \hat{\lambda}_2(t_1) > 0 \), we obtain \( \lambda_1(t_1) = \lim_{t \to t_1^+} \frac{\lambda_1(t)}{t - t_1} \leq 0 \). On the other hand, (8) implies \( \lambda_1(t_1) > 0 \), which is a contradiction. The same conclusion holds if \( t_1 \) is such that \( \lambda_1(t_1) > 0 \) and
$\lambda_2(t_1) = 0$. Hence, we can exclude this case.

Case b. Let $t_0 > 0$ the first time where $\phi(t_0) = 0$. If there exists a time $t_1 \in (0, t_0]$ such that $\lambda_1(t_1) < 0$ and $\lambda_2(t_1) \leq 0$, then we obtain a contradiction as we have $u = 0$ on $[0, t_0]$. Similarly, if there exists a time $t_1' \in (0, t_0]$ such that $\lambda_1(t_1') > 0$ and $\lambda_2(t_1') > 0$, then we obtain also a contradiction by the previous case. It follows that $\lambda_1 < 0$ and $\lambda_2 > 0$ on $[0, t_0]$. Assume that the trajectory is switching in $C$, so that $\mu_2'(s(t_0)) < \mu_2(s(t_0))$. Using that $\lambda_1(t_0) < 0$, we obtain:

$$\lambda_1(t_0)x_1(t_0)\mu'_2(s(t_0)) > \lambda_1(t_0)x_1(t_0)\mu_2(s(t_0)),$$

hence:

$$\dot{\phi}(t_0) < [x_1(t_0) + x_2(t_0)]\phi(t_0)\mu'_2(s(t_0)) \leq 0,$$

where the second inequality follows from the fact that $\phi = -\lambda_1 x_1 - \lambda_2 x_2 \leq 0$ on $[0, t_0]$. As $t_0$ is a switching point, we necessarily have $\phi(t_0) \geq 0$ which gives a contradiction. Hence, the trajectory switches at time $t_0$ in $A \cup B \cup D$ and $s(t_0) < \delta$. Now, Lemma 4 implies that $\lambda_1(t_0) > 0$ and $\lambda_2(t_0) < 0$, which contradicts case b. Hence, only case c is possible which proves (i). The proof of (ii) is straightforward from (i). Indeed, if $\lambda_1$ becomes negative on $(0, t_0)$, we obtain a contradiction as $u = 0$ over $[0, t_0]$. If $\lambda_2$ becomes positive, we can use case a) to eliminate this possibility.

**Lemma 7** Let us consider an optimal trajectory starting from $(x^0_1, x^0_2) \in A \cup B \cup C$, and suppose $\phi(0) > 0$.

(i) Then, we have $\lambda^0_1 < 0$ and $\lambda^0_2 > 0$.

(ii) If $[0, t_0)$ is the maximum time interval where $\phi > 0$, then $\lambda_1(t) < 0$ and $\lambda_2(t) > 0$ for any $t \in [0, t_0)$.

**Proof.** Similarly as in the proof of Lemma 6, we consider the three following cases: $\lambda^0_1 < 0$ and $\lambda^0_2 < 0$ (case a), $\lambda^0_1 > 0$ and $\lambda^0_2 < 0$ (case b), $\lambda^0_1 < 0$ and $\lambda^0_2 > 0$ (case c). The transversality condition implies that there exists a time $t' > 0$ such that $\phi(t') = 0$.

Case a. Let $t_0 > 0$ be the first time where $\phi(t_0) = 0$. At time $t_0$ both $\lambda_1(t_0)$ and $\lambda_2(t_0)$ are of distinct sign. It follows that either $\lambda_1$ or $\lambda_2$ is vanishing on $[0, t_0]$. First, assume that there exists $t_0' < t_0$ such that $\lambda_1(t_0') = 0$, $\lambda_1 < 0$ on $[0, t_0')$ and $\lambda_2 < 0$ on $[0, t_0')$. It follows that $\lambda_1(t_0') \geq 0$ which is in contradiction with (8) at time $t_0'$. We obtain a similar contradiction by changing the role of $\lambda_1$ and $\lambda_2$ which excludes this case.

Case b. First, notice that we have $\lambda_1 > 0$ and $\lambda_2 < 0$ on $[0, t_0]$. Indeed, if $\lambda_1$ is vanishing at a time $t_0' < t_0$ with $\lambda_2(t_0') < 0$, then we get a contradiction by the previous case. Also, both $\lambda_1$ and $\lambda_2$ cannot be positive on $[0, t_0]$ (as we have $u = 1$ on $[0, t_0]$). It follows that $\lambda_1$ and $\lambda_2$ remain of constant sign on $[0, t_0]$. As in the proof of the previous lemma, the trajectory remains in $A \cup B \cup C$ in the interval $[0, t_0]$ (eventually it reaches the target at time $t_0$ if it starts from $B$). Hence, we have $\mu_2'(s(t_0)) > \mu'_1(s(t_0))$ at time $t_0$ so that:

$$\psi(t_0) < (\lambda_1(t_0)x_1(t_0) + \lambda_2(t_0)x_2(t_0))\mu_2(s(t_0)) \leq 0,$$

where the second inequality follows from the fact that $\phi \geq 0$ on $[0, t_0]$. This gives $\phi(t_0) > 0$ which is in contradiction with the fact that $t_0$ is a switching point (implying $\phi(t_0) \leq 0$). It follows that only case c is possible which proves (i). The proof of (ii) is straightforward from (i). Indeed, if $\lambda_1$ becomes positive, then we have a contradiction with the sign of $\phi$ on $[0, t_0]$. Similarly, if $\lambda_2$ becomes negative, we have a contradiction by case a.

We now study initial conditions in $A \cup B \cup C$.

**Proposition 8** Consider an optimal trajectory starting in $A \cup B \cup C$. Then, there exists a time $t_0 > 0$ such that $u = 0$ over $[0, t_0]$. Moreover, either the trajectory reaches the target at time $t_0$, or it reaches the singular arc.

**Proof.** We first consider an initial condition in $B$. Assume that the trajectory contains an arc $u = 1$ on some time interval $[t_1, t_2]$ before reaching $\pi$. It follows that the trajectory remains in $B$ on this interval. Without any loss of generality, we may assume that $t_2$ is either the terminal time or a switching point, so that $\phi(t_2) = 0$. The previous Lemma implies that $\lambda_1 < 0$ and $\lambda_2 > 0$ on this interval which is in contradiction with Lemma 4. This proves that the trajectory cannot contain an arc $u = 1$ before reaching either the target or the singular arc as was to be proved.

We now consider an initial condition in $A \cup C$. Let us denote by $x$ an optimal trajectory starting from $(x^0_1, x^0_2)$ and by $u$ the associated optimal control. It is enough to show that the trajectory does not contain an arc $u = 1$ before reaching the target or the singular arc. Suppose that there exists a time interval $[t_1, t_2]$ such that $u = 1$ and $x(t) \in A \cup B \cup C$ for $t \in [t_1, t_2]$. If at time $t_2$, the trajectory is in $B$, we can conclude by the previous proposition. Otherwise, we have $x(t_2) \in A \cup C$, and without any loss of generality, we can assume that $t_2$ is a switching point so that $\phi(t_2) = 0$ (if the trajectory has no switching points for $t \geq t_2$, it does not reach the target). For $t \in (t_1, t_2)$, we have $\lambda_1(t) < 0$ and $\lambda_2(t) > 0$ from Lemma 7. Now, at time $t_2$, the trajectory switches to $u = 0$, so that by Lemma 6 there exists a time interval $[t_2, t_3]$ such that we have $\lambda_1(t) > 0$ and $\lambda_2(t) < 0$. As both $\lambda_1$ and $\lambda_2$ cannot vanish at the same time, we obtain a contradiction. Hence, we have $u = 0$ as was to be proved.

We now study initial conditions in $D$. 

Proposition 9 Consider an optimal trajectory starting at \((x_1^0, x_2^0) \in D\). Then, there exists a time \(t_0 > 0\) such that \(u = 1\) over \([0, t_0]\), and either the trajectory reaches the target at time \(t_0\) or it reaches the singular arc. Moreover, in the latter case we have \(s(t) = \hat{s}\) for any \(t \in [t_0, t_f]\).

PROOF. Assume that we have \(\phi(0) < 0\) at time 0. The transversality condition guarantees the existence of a time \(t_0 > 0\) such that \(\phi(t_0) = 0\), and we necessarily have \(\phi(t_0) \geq 0\). At time \(t_0\), the trajectory is in \(D\), hence combining (13) with the expression of \(\phi\) gives:

\[
\dot{\phi}(t_0) = -\frac{\left[x_1(t_0) + x_2(t_0)\right]\left[\mu'_1(s(t_0)) - \mu'_2(s(t_0))\right]}{\mu_1(s(t_0)) - \mu_2(s(t_0))} < 0,
\]

which gives a contradiction. It follows that the trajectory satisfies \(u = 1\) for all time \(t\) until reaching the target or the singular arc \(\Delta_{SA}\). Now, if the trajectory leaves the singular arc with the control \(u = 1\), we obtain a contradiction by the previous proposition. Similarly, the trajectory cannot leave the singular arc before reaching the target with the control \(u = 0\) (by repeating the argument above and (20)). The conclusion of the proposition follows.

Theorem 2 Under hypothesis 1, 2 and 3, system (5) satisfies the following property. For any initial condition \((x_1^0, x_2^0) \in E\), the optimal feeding strategy steering \((x_1^0, x_2^0)\) to the target is the feedback control law provided by (17) (see Fig. 2).

PROOF. Choose an initial condition in \(A \cup B \cup C\). Then Proposition 8 implies that an optimal trajectory necessarily satisfies \(u = 0\) until reaching the target or the singular arc. If the trajectory reaches the singular arc \(\Delta_{SA}\) before the target, we conclude by Proposition 9. If now, the initial point is in \(D\), we conclude again by Proposition 9.

The optimal strategy \(SAS_7\) consists in the regulation of the substrate, that is an auxostat. In the invariant manifold, it also corresponds to the regulation of the total biomass (turbidostat). These operating modes are known to select the fastest growing species (see e.g. [5]). Here, quite naturally, we have shown that the auxostat is optimal when the set-point is chosen as the maximum of the difference between the growth rate of both species. For a practical implementation of such strategy, the main challenge will be to estimate this set-point since the growth rates are generally poorly known.

4.3 Optimal synthesis in the case of \(T_2\)

We now discuss the case where the target is given by \(T_2\). One can see from (19) that \(\dot{p} > 0\) whenever \(s < \hat{s}\) which implies that the target cannot be reached at some point \(x\) such that \(s < \hat{s}\). It follows that for any initial point in \(E\) such that \(s_0 < \hat{s}\), the only possibility for the trajectory to reach the target is to cross \(s = \hat{s}\). In particular, whenever Hypothesis 3 is not satisfied, the target cannot be reached from any point in \(E\). By similar arguments as for \(T_1\), one can prove the following result.

Theorem 3 Under hypothesis 1, 2 and 3, the optimal feedback control in order to reach \(T_2\) is \(u = 1\).

In this case, the optimal strategy tends to wash-out the biomass. The target can be modified (e.g. adding a constraint on the total biomass) in order to avoid such effect.
4.4 Study of the problem outside of $F$

In this section, we briefly discuss the case where initial conditions $\xi_0 := (x_0^1, x_0^2, s_0)$ are outside the set $F$. We define two sets $F^\pm \subset \mathbb{R}^3$ by:

$$F^+ := \{ (x^1, x^2, s) \in \mathbb{R}^*_+ \times \mathbb{R}^*_+ \times (0, s_{in}) \mid x^1_0 + x^2_0 + s_0 > s_{in} \},$$

and $F^-$ is similarly defined with the reverse inequality.

Both sets $F^\pm$ are invariant by (1) using (3). If we let $M_0 := M(0)$ (recall (3)), then $M_0 < s_{in}$ (resp. $M_0 > s_{in}$) implies $M(t) < s_{in}$ (resp. $M(t) > s_{in}$) for all $t \geq 0$. In this setting, the target is a subset of $\mathbb{R}^3$ and is given by:

$$\mathcal{T}' := \{(x_1, x_2, s) \in \mathbb{R}^*_+ \times \mathbb{R}^*_+ \times (0, s_{in}) \mid x_2 \leq \varepsilon x_1 \}.$$

Notice that no assumption is required on the substrate concentration at the terminal time. The minimal time problem becomes:

$$\min_{u \in \mathcal{U}} (t(u)) \text{ s.t. } (x_1(t(u)), x_2(t(u)), s(t(u))) \in \mathcal{T},$$

where $(x_1, x_2, s)$ is the solution of (1) with $x_1(0) > 0$, $x_2(0) > 0$ and $s(0) \in (0, s_{in})$, and $t(u)$ is the first entry time into the target. The next proposition characterizes singular arcs for problem (21).

Proposition 10 Let us consider a singular arc defined on some time interval $[t_1, t_2]$.

(i) Then, $s$ is constant on the interval $[t_1, t_2]$.

(ii) If $M_0 < s_{in}$ and $s < \hat{s}$, the singular arc is controllable and we have $\dot{x}_1 > 0$ along the singular arc.

(iii) If the target is reached on $[t_1, t_2]$, then $s(t) = \bar{s}$.

PROOF. We apply Pontryagin maximum principle to (21). The Hamiltonian $H = H(x_1, x_2, s, \lambda_1, \lambda_2, \lambda_s, 0, u)$ for this problem can be written as follows:

$$H = [\lambda_1 - \lambda_s] \mu_1(s)x_1 + [\lambda_2 - \lambda_s] \mu_2(s)x_2 + \lambda_0 + u[-\lambda_1x_1 - \lambda_2x_2 + \lambda_s(s_{in} - s)].$$

If $u$ is an optimal control and $z := (x_1, x_2, s)$ is the corresponding trajectory, there exists $t_f > 0$, $\lambda_0 \leq 0$ and an absolutely continuous mapping $\lambda = (\lambda_1, \lambda_2, \lambda_s) : [0, t_f] \rightarrow \mathbb{R}^3$ such that $(\lambda_0, \lambda(t)) \neq 0$, and satisfying the adjoint equation:

$$\begin{align*}
\dot{\lambda}_1 &= -[(\lambda_1 - \lambda_s) \mu_1(s) - \lambda_1 u], \\
\dot{\lambda}_2 &= -[(\lambda_2 - \lambda_s) \mu_2(s) - \lambda_2 u], \\
\dot{\lambda}_s &= -[(\lambda_1 - \lambda_s)x_1 \mu'_1(s) + (\lambda_2 - \lambda_s)x_2 \mu'_2(s) - u \lambda_s].
\end{align*}$$

By deriving the switching function $\varphi := -\lambda_1x_1 - \lambda_2x_2 + \lambda_s(s_{in} - s)$, we find:

$$\dot{\varphi} = -[s_{in} - s][\lambda_1x_1 \mu'_1(s) + (\lambda_2 - \lambda_s)x_2 \mu'_2(s)].$$

Assume now that an extremal trajectory contains a singular arc on some time interval $[t_1, t_2]$. Hence, we have $\varphi = 0$ over this interval, that is:

$$-\lambda_1x_1 - \lambda_2x_2 + \lambda_s(s_{in} - s) = 0$$

By deriving, we have $\dot{\varphi} = 0$, hence $\ddot{\varphi} = 0$ (23) gives $\lambda_1 - \lambda_s)x_1 \mu'_1(s) + (\lambda_2 - \lambda_s)x_2 \mu'_2(s) = 0$ on this interval, that is:

$$\lambda_1 - \lambda_s)x_1 \mu'_1(s) + (\lambda_2 - \lambda_s)x_2 \mu'_2(s) = 0.$$

By deriving (23) on $[t_1, t_2]$, we obtain after some simplifications:

$$[(\lambda_1 - \lambda_s)x_1 \mu''_1(s) + (\lambda_2 - \lambda_s)x_2 \mu''_2(s)]s = 0.$$

Assume that $s$ is non-zero on $[t_1, t_2]$. Combining (23) and (24) gives $\lambda_1 - \lambda_s = \lambda_2 - \lambda_s = 0$. Now, (22) rewrites $-(\lambda_1 - \lambda_s)x_1 - (\lambda_2 - \lambda_s)x_2 + \lambda_s(s_{in} - s - x_1 - x_2) = 0$, and using that $H_+$ and $H_-$ are invariant, we obtain $\lambda_s = 0$ so that $\lambda = 0$. Hence, we have a contradiction which proves (i). To prove (ii), notice that the singular control can be written:

$$u_s = \frac{\mu_1(s)x_1 + \mu_2(s)x_2}{s_{in} - \dot{M} + x_1 + x_2},$$

hence, we conclude that $u_s \in [0, 1]$ provided that $s_{in} - M_0 > 0$ as was to be proved. Substituting $u = u_s$ into the initial system yields

$$\begin{align*}
\dot{x}_1 &= \frac{x_1}{s_{in} - s} [\mu_1(s)x_2 + \mu_1(s)(s_{in} - M)], \\
\dot{x}_2 &= \frac{x_2}{s_{in} - s} [\mu_2(s)x_1 + \mu_2(s)(s_{in} - M)].
\end{align*}$$

Thus, $s_{in} - M_0 > 0$ together with $s < \hat{s}$ implies that $\dot{x}_1 > 0$. To prove (iii), let us write the transversality conditions associated to (21). As $s(t_f) = 0$, we have $\lambda_s(t_f) = 0$, and similarly as for (6), we have at time $t_f$:

$$\lambda_1(t_f)x_1(t_f) + \lambda_2(t_f)x_2(t_f) = 0.$$
time steps, constant initialization, and a tolerance for IPOPT NLP solver set at $10^{-14}$.

The two solutions are obtained whenever the initial substrate concentration is chosen greater than $\bar{s}$ (see Fig. 3) and less than $\bar{s}$ (see Fig. 4). Corresponding parameter values are given in Table 2 in the space $(x_1, p, s)$ (recall (18)). The control provided by this method is of the form $(0, u_\pi)$ in Fig. 3 and of the form $(1, u_\pi)$ in Fig. 4 which confirms Remark 11.

### Table 2

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<th>$k_1$</th>
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<th>$k_2$</th>
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Values of the parameters (arbitrary units) in Fig. 3 (first row) and 4 (second row) with $\mu_1$ and $\mu_2$ given by (2).

growth rates are Haldane functions for example. Here, we present the study of problem (6) in the case of three extrema, i.e. when Hypothesis 1 is replaced by the following.

### Hypothesis 4

The growth functions of the two species fulfill the following conditions (see Fig. 5):

- there exist $\hat{s}_2 > \hat{s}_1 > 0$ such that $\mu_1(\hat{s}_i) = \mu_2(\hat{s}_i)$, $i = 1, 2$.
- the function $s \mapsto \mu_1(s) - \mu_2(s)$ has exactly two maxima for $s = \bar{s}_1$ and $s = \bar{s}_2$, and one minimum for $s = \bar{s}$, with $\bar{s}_1 < \hat{s}_1 < \bar{s} < \hat{s}_2 < \bar{s}_2$.

In this setting, we can define three singular arcs associated to $\bar{s}_1$, $\bar{s}_2$ and $\hat{s}$. Following the proof of Theorem 2, we can infer that the singular arc strategy $SAS_{\bar{s}}$ is optimal for reaching $T_3$. The situation is more delicate for the target $T_1$ since there exist two singular strategies associated to $SAS_{\bar{s}_1}$ and $SAS_{\bar{s}_2}$ which are candidates to

5 Extension to other growth functions

In this section, we are interested in the optimal control problem when the function $s \mapsto \mu_1(s) - \mu_2(s)$ has more than one extremum. This situation can occur when both

![Fig. 3](image1.png)

![Fig. 4](image2.png)

![Fig. 5](image3.png)
reach the target. Such competition between two singular arcs have already appeared in the minimal time control problem of fed-batch bioreactor for growth function with two maxima (see [1,7]). Following [1], we infer that an optimal control cannot switch from a singular arc to another one, and that the following conjecture holds true.

**Conjecture 12** Under hypothesis 2, 3 and 4, system (5) satisfies the following property. For any initial condition $\left(x_1^0, x_2^0\right) \in E$, the optimal feeding strategy steering $\left(x_1^0, x_2^0\right)$ to the target $T_1$ is either the singular arc strategy $\text{SAS}_{s_1}$ or the singular arc strategy $\text{SAS}_{s_2}$.

We compare numerically the time to reach the target $T_1$ with the singular arc strategies $\text{SAS}_{s_1}$ and $\text{SAS}_{s_2}$. This allows us to define a curve where both strategies are equivalent (see Fig. 6). This curve delimits two regions where each singular strategy is better than the other one, and so probably optimal.

![Fig. 6. Optimal trajectories (in red) to reach the target $T_1$ (green line) for growth functions satisfying Hypothesis 4 (see Fig. 5) in the $(s,p)$ plan. Dashed line: singular arc $\Delta_{s_{A_1}}$ (i.e. $s = \bar{s}_t$). The level curves represent the relative difference between the two singular arc strategies $\text{SAS}_{s_1}$.](image)

6 Conclusions and perspectives

In this work, we have proposed an alternative approach to the competitive exclusion principle using a singular strategy for selecting in a two-species chemostat model the one of interest. Our method relies on Pontryagin maximum principle and the exclusion of extremal trajectories. We believe that this kind of strategy can be the basis for future developments of species selection in chemostat. In particular, it could be interesting to study the more delicate situations with three or more species, or in presence of biotic interaction.

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**References**


