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# Geometric Optimal Control Techniques to Optimize the Production of Chemical Reactors using Temperature Control

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## Abstract

The dynamics of mass reaction kinetics chemical systems is modeled by the Feinberg-Horn-Jackson graph and under the "zero deficiency assumption", the behavior of the solutions is well known and splits into two cases: if the system is not weakly reversible there exists no equilibrium, nor periodic solution and if the network is weakly reversible in each stoichiometric subspace there exists only one equilibrium point and this point is asymptotically stable. By varying the temperature, one gets a single input control system and in this article we study the problem of maximizing the production of one species during the batch time. Our aim is to present the geometric techniques and results based on the Pontryagin maximum principle to compute the closed loop optimal solution. The complexity of the problem is illustrated by using two test bed examples: a sequence of two irreversible reactions and the McKeithan scheme.

*Keywords:* Mass action chemical systems, Zero deficiency theorem, Pontryagin maximum principle, Geometric optimal control

## 1. Introduction

Important developments in optimal control come from the Pontryagin maximum principle [28] which combined later (in the eighties) with the geometric techniques led to seminal theoretical results, see for instance [1] and [19]. They were applied to many industrial problems in space mechanics, quantum control [12] and an important modern application is the control of biological and chemical systems [29].

The objective of the article is to present the techniques of this area to analyze the problem of maximizing the production of one chemical species $[X]$ of a chemical network where the sequence of reactions occurs in a batch chemical reactor and the control is the temperature. Thanks to the Maximum Principle it can be formulated as minimizing the batch time $t_f$ to produce a fixed amount $[X] = d$ and this leads to a time minimal control problem for a single input control system: $\frac{\mathrm{d}c}{\mathrm{d}t} = f(c, T)$, where $c$ is the concentrations vector, $T$ is the temperature, with $c(0) = c_0$ and $c(t_f) \in N$, $N$ being the terminal manifold: $\{[X](t_f) = d\}$. The dynamics model under the mass action kinetics assumption produces, at constant temperature $T$, a polynomial system, which can

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be deduced from the Feinberg-Horn-Jackson graph [32]. Thanks to the so-called seminal zero deficiency theorem obtained by the contributions of Feinberg, Horn, Jackson in the $70's$, the behaviors of solution can be split in many applications into two cases. The first case is the non weakly reversible case, and there exists no equilibrium point nor periodic trajectory, an example being a sequence of consecutive reactions $A \to B \to C \ldots$. The second case is the weakly reversible case, where under a mild additional assumption, in each stoichiometric class there exists an unique equilibrium point $c^*$ which is asymptotically stable, see [17, 20]. An example of this case being the so-called McKeithan scheme: $T + M \rightleftarrows A \longrightarrow B$ .

If the dynamics is simple at fixed temperature, the optimal control by varying the temperature can be very complicated as illustrated by the following tutorial example. The rate of each reaction using *Arrhenius law* depends upon $k(T) = A\, e^{-E/(RT)}$ where $A, E$ are parameters, the second $E$ being the *energy of activation*. Consider the following scheme $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ of a sequence of two first order irreversible reactions. Denoting by $c_1 := [A]$, $c_2 := [B]$ the respective concentrations, the dynamics takes the form:

$$\dot{c}_1 = -k_1 c_1,\ \dot{c}_2 = k_1 c_1 - k_2 c_2,\ k_i = A_i\, e^{-E_i/(RT)}, i = 1, 2.$$

Since $T \mapsto v(T) := k_1(T)$ is a bijection, $v$ can be chosen as the control variable. The dynamics is irreversible and is very simple (note it is a consequence of the zero deficiency theorem) and integrating the dynamics at constant temperature leads to two situations only: $k_1 \neq k_2$ or $k_1 = k_2$ (resonant case). But assume that we want by controlling the temperature to maximize the ratio: $z = c_2/c_1$. This leads to maximize $z(t_f)$ where $[0, t_f]$ is the batch duration. Using the dynamics: $\dot{z} = v - \beta v^\alpha z + vz$, $\alpha = E_2/E_1$, $\beta = A_2/A_1^\alpha$ with $z(0) = [B]/[A]_{|t=0}$ which can be taken as $z(0) = 0$ and $v \in [v_m, v_M]$ is associated to $T \in [T_m, T_M]$. Denoting $H = \dot{z}$ (which plays the role of Hamiltonian in the optimal problem) the problem leads to maximize $H$ over $v \in [v_m, v_M]$ in order to maximize $z(t_f)$. Clearly one gets three cases if $\alpha > 1$ (and one case if $\alpha < 1$): the maximum is depending upon $z$ and can be either $v = v_m$, $v = v_M$ or an intermediate value $v = v_s$ called singular in optimal control defined by: $\frac{\partial H}{\partial v} = 1 - \alpha\beta v^{\alpha-1} z + z = 0$.

In this case a simple graph analysis of $H$ tells us that an optimal policy can be of the form $\sigma_M \sigma_s \sigma_m$ where $\sigma_M, \sigma_s, \sigma_m$ being arcs associated to $v_M, v_s, v_m$ respectively, $\sigma_1\sigma_2$ representing an arc $\sigma_1$ followed by $\sigma_2$. This corresponds on $[0, t_f]$ to the concatenation of the controls $v_M, v_s, v_m$.

A similar analysis in the case of $\alpha < 1$ leads to the optimal control: $v = v_M$ over $[0, t_f]$, associated to maximal temperature $T_M$.

From this example we deduce two facts. The first one is that the optimal policy depends upon $\alpha = E_2/E_1$ v.s. $k_1/k_2$ for the dynamics at constant $T$. Second, the discussion depends upon the competition between the Hamiltonians $H$ associated to $v_m, v_M, v_s$, to provide the maximum of $H$. This second point will give the geometric frame to perform the analysis in relation with singularity theory: competition between Hamiltonians dynamics to compute the optimal solutions, see the earliest seminal contributions [16, 22]. In particular, the complexity of the problem is directly illustrated by the two test bed cases.

The organization of the article is the following. In section 2, the mathematical model is recalled based on the Feinberg-Horn-Jackson graph and the zero deficiency theorem is precisely stated [17, 20] and we present the two test bed cases, in particular the McKeithan network [30, 27]. The section 3 is devoted to the Pontryagin maximum principle and the classification of the solutions into regular and singular solutions. The general properties are discussed, based on [22] in the regular case and [8] in the singular case. This leads to compute time optimal sequences useful in our study, based on basic concepts of singularity theory, in particular semi-normal forms [26]. The section 4 presents the main technical tool to handle the problem that is singularity theory and classification of the optimal syntheses based on [10, 9]. This is applied in section 5 to discuss the optimal syntheses for the two test bed cases. In the final section we discuss in conclusion the mathematical and computational obstacles to complete our study.

## 2. Mathematical model and the zero deficiency theorem

In this section, we make a brief presentation of the model with main properties based on the seminal works of Feinberg-Horn-Jackson in the 70's. For more details, references are the earliest articles [17, 20] and [30, 2] for more recent contributions.

### *2.1. Mass action kinetics and the Feinberg–Horn–Jackson graph*

We consider a set of $m$ chemical species $\{X_1, \ldots, X_m\}$, and the state of the dynamics is the vector $c = (c_1, \ldots, c_m) \in \mathbb{R}^m_{\geq 0}$ representing the molar concentrations. Let $\mathcal{R}$ be a set of reactions, each reaction being denoted $y \to y'$ and is of the form:

$$\sum_{i=1}^{m} \alpha_i X_i \to \sum_{i=1}^{m} \beta_i X_i \ ,$$

where $\alpha_i$,$\beta_i$ are the *stoichiometric coefficients* and the vectors $y = (\alpha_1, \ldots, \alpha_m)^\intercal$ and $y' = (\beta_1, \ldots, \beta_m)^\intercal$ are forming the vertices of the so-called Feinberg-Horn-Jackson oriented graph associated to the network, edges being oriented according to $y \to y'$. Each reaction $y \to y'$ is characterized by a reaction rate $K(y \to y')$ and the system is said *simple* (or mass kinetics) if the rate of the reaction is of the form:

$$K(y \to y') = k(T)\, c^y, \tag{1}$$

$$c^y = {c_1}^{\alpha_1} \ldots {c_m}^{\alpha_m} \tag{2}$$

and

$$k(T) = A e^{-E/(RT)} \tag{3}$$

is the *Arrhenius law*, $A$ is the exponential factor, $E$ is the activation energy, both depending on the reaction, $R$ is the gas constant and $T$ is the temperature. Note that another rate formulae can be used in particular to deal with biomedical systems (see for instance [30]). One can label the sequences of reaction $\mathcal{R}$ by $i = 1, \ldots, \tilde{n}$ and this is defining a set of (increasing) functions of the temperature denoted $k_i(T), i = 1 \ldots \tilde{n}$, each defined by a set of parameters $(A_i, E_i)$ forming the set $\Lambda$.

The dynamics of the system, taking into account the whole network is:

$$\dot{c}(t) = f(c(t), T) = \sum_{y \to y' \in \mathcal{R}} K(y \to y')\,(y' - y). \tag{4}$$

Note that if the reactor is fed at some constant rate $r$, the more general dynamics takes the form

$$\dot{c}(t) = f(c(t), T) + r\left((c_1^0, \ldots, c_m^0)^\intercal - c(t)\right). \tag{5}$$

where $(c_1^0, \ldots, c_m^0)$ are the fixed concentrations of the feeding reactor. This led to a more general system which can be set in an unique frame of chemical network (introducing additional reaction), but in this article, from the purpose of control theory, we shall consider only the case (4) which is called the *batch* (or closed) case.

*2.2. More explicit representation of the dynamics and the zero deficiency theorem*

First of all, we introduce the so-called *stoichiometric subspace* $S = \mathrm{span}\{y - y',\ y \to y' \in \mathcal{R}\}$ and the set $(c(0) + S) \cap \mathbb{R}^m_{\geq 0}$ are called the (strictly if $> 0$) *positive stoichiometric compatibility classes*. From (4) it is clear that $S$ is invariant for the dynamics but more precisely one has.

**Lemma 1** ([2]). *Let $c(t)$ be a solution of* (4) *with initial condition $c(0) \in \mathbb{R}^m_{>0}$. Then $c(t) \in \mathbb{R}^m_{>0}$ for all $t > 0$.*

Before to state our theorem the dynamics has to be rewritten using the following concepts.

- Having labeled the set of vertices by $i = 1, \cdots, n$, whose corresponding stoichiometric vectors $(y_1, \ldots, y_n)$, the *complex matrix* is $Y = (y_1, \ldots, y_n)$
- *The incidence connectivity matrix:* $A := (a_{ij})$ contains the Arrhenius coefficients $k_i$ of the reactions using the rule: $k_1 = a_{21}$ indicating a reaction with constant $k_1$ from the first node to the second, that is $y_1 \xrightarrow{k_1} y_2$ .

With the mass kinetics assumption (see [30] for extension) the dynamics (4) can be expressed as

$$\dot{c}(t) = f(c(t), T) = Y\tilde{A}\, c^Y \tag{6}$$

where $\tilde{A}$ is the *Laplacian matrix* in graph theory defined by

$$\tilde{A} = A - \mathrm{diag}\left(\sum_{i=1}^{n} a_{i1}, \ldots, \sum_{i=1}^{n} a_{in}\right) \tag{7}$$

and we denote:

$$c^Y = (c^{y_1}, \ldots, c^{y_n})^\intercal. \tag{8}$$

*2.3. Examples in the two test bed cases*

*Case 1: Sequence of N first order reactions.* $A \xrightarrow{k_1} B \xrightarrow{k_2} C\ \ldots$. Let $c = (c_1, \ldots, c_{N+1}) \in \mathbb{R}^{N+1}$ and the dynamics takes the form:

$$\begin{pmatrix} \dot{c}_1 \\ \vdots \\ \dot{c}_N \end{pmatrix} = \begin{pmatrix} -k_1 & 0 & \cdots & \cdots & 0 \\ k_1 & -k_2 & \ddots & 0 & \vdots \\ 0 & k_2 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & k_{N-1} & -k_N \end{pmatrix} \begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix}. \tag{9}$$

One can introduce the normalized concentration $c_i/(c_1(0) + \ldots + c_{N+1}(0))$, so that $c_i \in [0, 1]$. Observe also that the $c_{N+1}$ evolution can be deleted and this amounts to restrict to the stoichiometric class.

For the case $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ further normalizing coordinates are:

$$x = \ln c_1,\ y = c_2/c_1,\ v = k_1 \tag{10}$$

and the dynamics takes the form:

$$\dot{x} = -v,\ \dot{y} = v - \beta y v^\alpha + vy,\ \dot{v} = u, \tag{11}$$

where $\alpha = E_2/E_1,\ \beta = A_2/A_1^{\alpha}$.

Equations can be extended to a more general scheme:

$$n_1\, A \xrightarrow{k_1} n_2\, B \xrightarrow{k_2} n_3\, C \xrightarrow{k_3} \cdots$$

of $N$ consecutive irreversible reactions of order $n_i$. We obtain the following matrices:

$$Y = \mathrm{diag}(n_1, \ldots, n_{N+1}), \quad A = \begin{pmatrix} 0 & \cdots & \cdots & \cdots & 0 \\ k_1 & 0 & \cdots & \cdots & 0 \\ 0 & k_2 & 0 & \cdots & 0 \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ 0 & 0 & 0 & k_N & 0 \end{pmatrix}.$$

Introducing "reversibility" $A \underset{k_3}{\overset{k_1}{\rightleftarrows}} B \xrightarrow{k_2} C$ leads to

$$\begin{aligned} \dot{c}_1 &= -v c_1 + \beta v^{\alpha} c_2 \\ \dot{c}_2 &= v c_1 - \beta v^{\alpha} c_2 - \beta' v^{\alpha'} c_2 \end{aligned} \tag{12}$$

where $\alpha = E_3/E_1, \alpha' = E_2/E_1, \beta = A_3/A_1^{\alpha}, \beta' = A_2/A_1^{\alpha'}$.

*Case 2: McKeithan scheme ([30, 27]).* It is given by:

$$\begin{tikzcd} T + M \arrow[r, "k_1"] & C_0 \arrow[l, bend left, "k_{-1,0}"] \arrow[r, "k_{p,0}"] & C_1 \arrow[ll, bend left, "k_{-1,1}"] \arrow[r, "k_{p,1}"] & \cdots \arrow[r, "k_{p,N}"] & C_N \arrow[llll, bend left, "k_{-1,N}"] \end{tikzcd} .$$

The matrix $Y$ is defined by:

$$Y = \begin{pmatrix} 1 & 0 & \ldots & \ldots & 0 \\ 1 & 0 & & & \vdots \\ 0 & 1 & \ddots & & \vdots \\ \vdots & \ddots & \ddots & \ddots & \vdots \\ \vdots & & \ddots & 1 & 0 \\ 0 & \ldots & \ldots & 0 & 1 \end{pmatrix}$$

and the matrix $A = (a_{ij})$ is defined by: $a_{21} = k_1,\ a_{1,i} = k_{-1,i-2}\ i = 2, \ldots, m\ (m = N + 2)$, $a_{i,i-1} = k_{p,i-3}$, $i = 3, \ldots, m$ and all others $a_{i,j} = 0$.

The stoichiometric subspace is defined by $S = \{c\ ;\ T + C_0 + \ldots + C_N = M + C_0 + \ldots + C_N = 0\}$ and let $\delta_1 = T + C_0 + \ldots + C_N$ and $\delta_2 = M + C_0 + \ldots + C_N$ the constant associated to first integrals.

Consider the case $N = 2$ so that the reaction scheme is denoted

$\begin{tikzcd} T + M \arrow[r, "k_1"] & A \arrow[l, bend left, "k_3"] \arrow[r, "k_2"] & B \arrow[ll, bend left, "k_4"] \end{tikzcd}$ and restricting to the stoichiometric class ($\delta_1$ and $\delta_2$ fixed), one gets with

$x := [A]$, $y := [B]$ the dynamics

$$\begin{aligned} \dot{x} &= k_1\,(\delta_1 - x - y)(\delta_2 - x - y) - (k_2 + k_3)\,x \\ \dot{y} &= k_2\,x - k_4\,y. \end{aligned} \tag{13}$$

*2.4. The zero deficiency theorem [17, 20]*

*Definition and notation*. Using graph theory concepts we introduce the following: the *deficiency* of the network is: $\delta = n - l - s$, with $n$ = number of vertices, $l$ = number of connected components and $s$ = dimension of the stoichiometric subspaces. The network is called *weakly reversible* if for each pair $(i, j)$ of vertices such that there exists an oriented path joining $i$ to $j$ there exists a path joining $j$ to $i$.

**Theorem 1.** *Let any simple reaction network of deficiency zero.*

*(i) If the network is not weakly reversible, then for arbitrary kinetics, the differential equation cannot have a positive equilibrium nor a periodic trajectory that is contained in* $\mathbb{R}^m_{>0}$

*(ii) If the network is weakly reversible, there exists within each strictly positive stoichiometric compatibility class precisely one equilibrium* $c^*$*, the equilibrium is locally asymptotically stable with (pseudo-Helmholtz) Lyapunov function* $V(c, c^*) = \sum_i \left[c_i(\ln c_i - \ln c_i^* - 1) + c_i^*\right]$. *Moreover, there is no non trivial periodic orbit.*

**Remark 1.** *Note that additional properties in the McKeithan network led to global stability property (see [2]) and the proof of the existence of equilibrium related to the Perron-Frobenius therorem [30].*

**Application.**

- *Case 1* $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ : $\delta = 3 - 1 - 2 = 0$ and the network is not weakly reversible.
- *Case 2* $\begin{tikzcd} \mathrm{T+M} \arrow[r, "k_1"] & \mathrm{A} \arrow[r, "k_2"] \arrow[l, bend left, "k_3"] & \mathrm{B} \arrow[ll, bend left, "k_4"] \end{tikzcd}$ : $\delta = 3 - 1 - 2 = 0$. The network is weakly reversible.

  Equilibrium can be easily found from (13) by solving $\dot{x} = \dot{y} = 0$ and we get.

**Lemma 2.** *Let* $(\delta_1, \delta_2) \in {\mathbb{R}_+^*}^2$ *fixed. There exists a unique equilibrium point* $X_{eq} = (x^e, y^e) \in \mathbb{R}_+^2$ *for the system* (13) *given by*

$$x^e = \frac{2\delta_1\delta_2 k_1 k_4}{\Delta + \delta_p\,\alpha + \beta}, \quad y^e = \frac{2\delta_1\delta_2 k_1 k_2}{\Delta + \delta_p\,\alpha + \beta}$$

*where* $\alpha = k_1\,(k_2 + k_4)$*,* $\beta = k_4\,(k_2 + k_3)$*,* $\delta_m = \delta_1 - \delta_2$*,* $\delta_p = \delta_1 + \delta_2$ *and* $\Delta = \sqrt{\delta_m^2\alpha^2 + 2\delta_p\,\alpha\beta + \beta^2}$.

**Proposition 1.** *Take the equilibrium point* $X_{eq}$*. The linearized system at* $X_{eq}$ *is defined by the matrix*

$$L = \begin{pmatrix} \frac{-k_2(k_2+k_3)-\Delta}{k_2+k_4} & \frac{k_4(k_2+k_3)-\Delta}{k_2+k_4} \\ k_3 & -k_4 \end{pmatrix}.$$

*We have* $\det L = \Delta > 0$ *and* $\operatorname{Tr} L = -\left(\frac{\Delta + k_2(k_2+k_3)}{k_2+k_4} + k_4\right) < 0$*. The point* $X_{eq}$ *is globally asymptotically stable and*

- *if* $(\operatorname{Tr} L)^2 - 4\det L < 0$*, then* $X_{eq}$ *is a stable focus (see Fig.1 (left)),*
- *if* $(\operatorname{Tr} L)^2 - 4\det L > 0$*, then* $X_{eq}$ *is a stable node (see Fig.1 (right)).*

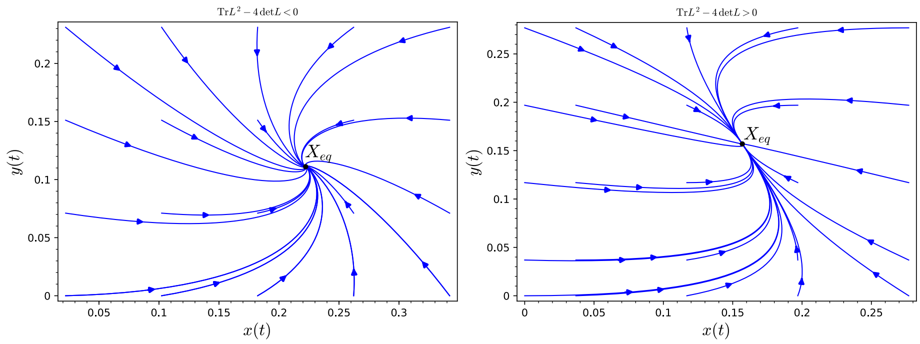


Figure 1: Phase portrait for the McKeithan model. (left) Focus; (right) Node.

## 3. Pontryagin maximum principle and extremal curves

### *3.1. Statement and notation for the optimal control problem*

The system is written as $\frac{\mathrm{dc}}{\mathrm{dt}} = f(c, T)$ and controlling the temperature leads to $T \in [T_m, T_M]$. In practice, thermodynamics has to be used to model the heat exchanges, in relation with the heat produce by the reactions [32] or the heat exchange model used in the experiments. To avoid this part of the study and without loss of generality for the mathematical point of view, we shall choose $\dot{v}$ as the control variable, where $v$ is defined by $v = k_i(T)$ for some reaction $i$. This leads to deal with the single-input affine control system:

$$\dot{q}(t) = F(q(t)) + u(t)\, G(q(t)) \tag{14}$$

where $q = (c, v) \in \mathbb{R}^n$, $F = F(c, v)\frac{\partial}{\partial c}$, $G = \frac{\partial}{\partial v}$, $u_- < u < u_+$ and the bounds $v \in [v_m, v_M]$ will not be taken into account. Note that the map : $v \mapsto \dot{v}$ is the standard *Goh-transformation* in optimal control and plays an important role (see [6]). We choose the labeling such that the optimization of the production is given by:

$$\max \ c_1(t_f) \tag{15}$$

where $t_f$ is the time duration of the batch time. An equivalent formulation will be (thanks to the maximum principle)

$$\min \ t_f, \quad c_1(t_f) = d,$$

where $d \geq 0$ is the desired amount of the species $[X_1]$ during the batch duration $t_f$.

### *3.2. Maximum principle [28]*

#### *3.2.1. Geometric preliminaries*

Consider a single-input control system: $\dot{q}(t) = f(q(t), u(t))$, $q \in \mathbb{R}^n$, $f$ real analytic and the set of input is the set $\mathcal{U}$ of bounded measurable mappings $u : [0, t_f(u)] \mapsto [-1, +1]$. Fixing $q(0) = q_0$ we denote by $q(\cdot, q_0, u)$ the solution associated to $u(\cdot)$ and starting from $q(0)$. The *accessible set* in time $t_f$ is the set: $A(q_0, t_f) = \cup_{u(\cdot)} q(t_f, q_0, u)$, image at time of the *extremity mapping*: $E^{q_0, t_f} : \mathcal{U} \ni u(\cdot) \mapsto q(t_f, q_0, u) \in \mathbb{R}^n$. The set of inputs is endowed with the $L^\infty$−norm topology. The Maximum Principle is a parametrization of the boundary of accessibility set.

*3.2.2. Needle or Weierstrass variations. First order Pontryagin cone $K_1(t_f)$*

Take $u(\cdot) \in \mathcal{U}$ such that the solution written shortly $q(\cdot)$ is defined on $[0, t_f]$ and let $t$ be a *Lebesgue time* on $[0, t_f]$. A *needle variation* of $u(\cdot)$ with data $(t, v, \varepsilon)$ is the $L^1$ perturbation defined by: $u_\varepsilon = v$ on $[t - \varepsilon, t]$ and equal to the control $u(\cdot)$ elsewhere with $\varepsilon > 0$ and $v$ *constant* $\in [-1, +1]$. We shall denote in short by $q_\varepsilon(\cdot)$ the response to $u_\varepsilon$ (starting at time 0 from $q_0$). Consider at final time $t_f$, the curve $\varepsilon \mapsto q_\varepsilon(t_f)$. The first order Pontryagin cone $K_1(t_f)$ is the smallest *convex closed cone* containing tangent vectors $\frac{\mathrm{d}}{\mathrm{d}\varepsilon}_{|\varepsilon=0} q_\varepsilon(t_f)$ for all perturbations. The key point of the Maximum Principle is to use the Pontryagin cone as an approximation of the accessibility set, see [28].

*3.2.3. Statement of the maximum principle*

One needs the following. The *pseudo-Hamiltonian* (or unmaximized Hamiltonian) is $H(q, p, u) = p \cdot f(q, u)$, where $p \in \mathbb{R}^n \backslash \{0\}$ is *the adjoint vector*. We denote $M(q, p) = \max_{|u| \leq 1} H(q, p, u)$.
Consider first the time minimal control problem, with $q(0) = q_0$ fixed and $q(t_f) \in N$: *terminal* analytic manifold. One has.

**Theorem 2.** *Assume $(q^*(\cdot), u^*(\cdot))$ is an optimal time minimal solution on $[0, t_f^*]$, then there exists $p^*(\cdot)$ nonzero such that a.e. on $[0, t_f^*]$*

$$\dot{q}^*(t) = \frac{\partial H}{\partial p}((q^*(t), p^*(t), u^*(t)), \tag{16a}$$

$$\dot{p}^*(t) = -\frac{\partial H}{\partial q}((q^*(t), p^*(t), u^*(t)) \tag{16b}$$

$$H((q^*(t), p^*(t), u^*(t)) = M((q^*(t), p^*(t)). \tag{16c}$$

*Moreover $t \mapsto M((q^*(t), p^*(t))$ is constant and non negative and at the final time one has the transversality condition:*

$$p^*(t_f) \perp T_{q^*(t_f)} N. \tag{17}$$

**Remark 2.** *If we replace the time minimal problem by a Mayer problem:*

$$\min_{u(\cdot)} \varphi(q(t_f)), \tag{18}$$

*the same conditions* (16a)*,* (16b)*,* (16c) *hold, while* (17) *is replaced by:*

$$p^*(t_f) = -\frac{\partial \varphi}{\partial q}(q^*(t_f)). \tag{19}$$

**Definition 1.** *An extremal triplet $(q, p, u)$ is a solution of* (16a)*,* (16b)*,* (16c) *and it is called a BC-extremal if the transversality condition is satisfied. An extremal control is called regular if $|u(t)| = 1$ a.e. and singular if $\frac{\partial H}{\partial u}(q, p, u) = 0$ everywhere. It is called exceptional if $M = 0$. A regular extremal is called bang-bang if the number of switches is finite.*

*3.2.4. Computation of singular extremals and properties*

*Notations.* Let $X, Y$ be two real analytic vector fields of $\mathbb{R}^n$, the *Lie bracket* is defined by: $[X, Y](q) = \frac{\partial X}{\partial q}(q)Y(q) - \frac{\partial Y}{\partial q}(q)X(q)$. The Hamiltonian lift of $X$ is $H_X(z) = p \cdot X(q),\ z = (q, p)$. The *Poisson bracket* is defined by $\{H_X, H_Y\}(z) = p \cdot [X, Y](q)$.

*Computation of singular extremals.*

**Definition 2.** *Let $H(z,u) = p \cdot f(q,u)$. The condition $\frac{\partial^2 H}{\partial u^2} \leq 0$ (resp $< 0$) is called (resp. strict) Legendre-Clebsch condition. Assume $f(q,u) = F(q) + u\,G(q)$. The condition $\frac{\partial}{\partial u}\frac{\mathrm{d}}{\mathrm{d}t^2}\frac{\partial H}{\partial u} = \{\{H_G, H_F\}, H_G\} \geq 0$ (resp. $> 0$) is called the (resp. strict) generalized Legendre-Clebsch condition.*

**Computation.** If the strict Legendre-Clebsch condition is satisfied one uses $\frac{\partial H}{\partial u} = 0$ to compute the singular control $\hat{u}(z)$ using the implicit function theorem. Plugging such $\hat{u}(z)$ in $H(z,u)$ leads to the *true Hamiltonian* denoted $\hat{H}(z)$. In the affine case, one has $\frac{\partial^2 H}{\partial u^2} = 0$ and we proceed as follows. The relation $\frac{\partial H}{\partial u} = 0$ leads to $H_G(z) = p \cdot G(q) = 0$. Deriving twice with respect to time along the extremal solution leads to:

$$
\begin{aligned}
&H_G(z) = \{H_G, H_F\}(z) = 0,\\
&\{\{H_G, H_F\}, H_F\}(z) + u\,\{\{H_G, H_F\}, H_G\}(z) = 0.
\end{aligned}
\tag{20}
$$

Assume $\{\{H_G, H_F\}, H_G\}(z) \neq 0$, the singular extremal is called of *order 2* and the singular control $u$ is computed as $\hat{u}(z)$, using relation (20). Plugging such $\hat{u}(z)$ into $H(z,u)$ leads to a true singular Hamiltonian denoted $H_s(z)$, one has:

**Lemma 3.** *Singular extremals of order 2 are the solutions of:*

$$
\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H_s}{\partial p}(z),\ \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H_s}{\partial q}(z) \tag{21}
$$

*with the constraints $H_G(z) = \{H_G, H_F\}(z) = 0$. Moreover in order to be admissible the singular control given by*

$$
u_s(z) = -\frac{\{\{H_G, H_F\}, H_F\}(z)}{\{\{H_G, H_F\}, H_G\}(z)} \tag{22}
$$

*has to satisfy the admissibility constraints $|u_s(z)| \leq 1$.*

**Definition 3.** *Let $(z,u)$ be a singular extremal of order 2 and $M = H_F = h$ the constant value of the Hamiltonian. The extremal is called exceptional if $h = 0$.*
*If $h > 0$, the extremal is called hyperbolic (resp. elliptic) if $\{\{H_G, H_F\}, H_G\} > 0$ (resp. $< 0$).*

*Time optimality status of singular extremals for the point to point problem.* ($N$: single point). One needs the following seminal results based on [21] and [8], see also [6] for a tutorial presentation.

**Proposition 2** (High-order maximum principle)**.** *The generalized Legendre-Clebsch condition is a necessary small time optimality condition.*

Further results need the following.

*Statement of the limit problem.* We consider the time minimal problem with fixed end-point for the affine system:

$$
\frac{\mathrm{d}q}{\mathrm{d}t} = F(q) + u\,G(q). \tag{23}
$$

The limit problem is the following:

- the constraints $|u| \leq 1$ on the control are relaxed and we admit a specific class of *impulse controls*. More precisely, a trajectory is a finite concatenations of arcs corresponding to bounded measurable controls and finite jumps in the $G$ direction. The set of admissible controls extending $\mathcal{U}$ is denoted $\mathcal{U}'$.

*Assumptions.* Consider the affine system $\dot{q} = F(q) + u\,G(q)$ ($u \in \mathbb{R}$) and let $(q, p, u)$ be an extremal of order 2 on $[0, t_f]$. Assume the following on $\mathcal{U} \subset \mathbb{R}^n$.

($H_0$) $F, G$ are linearly independent and the reference extremal curve $t \mapsto q(t)$ is one-to-one. Since the concept of singular-extremal is feedback invariant (see [4]) one may set $u \equiv 0$. Let us denote by $K_1(t) = \mathrm{span}\{\mathrm{ad}^k\ F \cdot G(q(t));\ k \in \mathbb{N}\}$ with $\mathrm{ad}\,F \cdot G = [F, G]$. Then it is known that $K_1(t)$ is the first-order Pontryagin cone along $q(\cdot)$ and the codimension is non zero.

Moreover let us then assume that:

($H_1$) $\forall t \in [0, t_f],\ K_1(t)$ is of codimension one and is spanned by the vectors: $\mathrm{ad}^k\ F \cdot G(q(t)),\ k = 0, \ldots, n-2$.

($H_2$) If $n \geq 3,\ \forall t \in [0, t_f], F(q(t)) \notin \mathrm{span}\{\mathrm{ad}^k F \cdot G(q(t));\ k = 0, \ldots, n-3\}$.

**Remark 3.** *Note* $\forall t \in [0, t_f],\ [[G, F], G](q(t)) \notin K_1(t)$.

**Theorem 3.** *Let $(q(\cdot), p(\cdot), u(\cdot))$ be a singular extremal defined on $[0, t_f]$ and satisfying assumptions $(H_1), (H_2)$. Note that the adjoint vector $p$ is then unique up to a non-zero factor, and for any time $t$ in $[0, t_f]$, $p(t)$ is orthogonal to $K_1(t)$; so $((q(t), p(t))$ is of order 2. Then there exists a $C^0$-neighborhood $U$ of the reference trajectory $q(\cdot)$ such that $q(\cdot)$ is a time-minimizing (resp. maximizing) trajectory with respect to all solutions of (23) contained in $U$ and joining $q(0)$ to $q(t_f)$ (the set of admissible control being $\mathcal{U}'$) if $(q(\cdot), p(\cdot), u(\cdot))$ is exceptional or hyperbolic (resp. elliptic) and if $t_f < t_{1c}$ where $t_{1c}$ is the first conjugate time to $t_f$ along $q(\cdot)$.*

*Proof.* See [8]. □

*Algorithm to compute conjugate times.* They are described in [5] and practically implemented in the software HamPath [15].

*Relation between affine and non affine case using the Goh transformation for chemical networks.* Recall that for our network: $\dot{c} = f(c, v),\ \ v = k_i$ is extended into $\dot{q} = F(q) + u\,G(q),\ \ F = f(c, v)\,\frac{\partial}{\partial c},\ \ G = \frac{\partial}{\partial v}$ with $q = (c, v)$. Denote $\tilde{H} = p_c \cdot f(c, v)$ and $H = p \cdot (F(q) + u\,G(q))$, $p = (p_c, p_v)$. One has the following relation between the corresponding singular extremals.

**Lemma 4.** *The pair $(q, p)$ is solution of:*

$$\dot{q} = \frac{\partial H}{\partial p},\ \ \dot{p} = -\frac{\partial H}{\partial q},\ \ \frac{\partial H}{\partial u} = 0$$

*if and only if $p_v = 0$ and $(c, p_c, v)$ is solution of:*

$$\dot{c} = \frac{\partial \tilde{H}}{\partial p_c},\ \ \dot{p}_c = \frac{\partial \tilde{H}}{\partial \tilde{c}},\ \ \frac{\partial \tilde{H}}{\partial v} = 0$$

*and moreover the following relations are satisfied*

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial H}{\partial u} = \{H_G, H_F\} = -\frac{\partial \tilde{H}}{\partial v} \tag{24}$$

$$\frac{\partial}{\partial u}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\frac{\partial H}{\partial u} = \{\{H_G, H_F\}, H_G\} = -\frac{\partial^2 \tilde{H}}{\partial v^2}. \tag{25}$$

In particular (25) relates the Legendre-Clebsch and the generalized Legendre-Clebsch condition of both systems.

*Computation in small dimensions.*

- $n = 2$. Note $q = (x, y)$. Introduce the following determinants

$$\begin{aligned} D &= \det(G, [[G, F], G]), \\ D' &= \det(G, [[G, F], F]) \\ D'' &= \det(G, F),\ \ D_s = \det(G, [G, F]). \end{aligned}$$

  Eliminating $p$ leads to:

  - S: Singular arcs located in $D_s = 0$.
  - Singular control: $u_s(q) = -D'(q)/D(q)$.
  - Hyperbolic: $DD'' > 0$.
  - Elliptic: $DD'' < 0$.

- $n = 3$. Note $q = (x, y, z)$. Introduce the following determinants:

$$\begin{aligned} D &= \det(G, [G, F], [[G, F], G]), \\ D' &= \det(G, [G, F], [[G, F], F]) \\ D'' &= \det(G, [G, F], F). \end{aligned}$$

  Eliminating $p$ leads to:

  - Singular control: $u_s(q) = -D'(q)/D(q)$.
  - Singular vector fields: $\dot{q} = F(q) - \frac{D'(q)}{D(q)} G(q)$.
  - Hyperbolic: $DD'' > 0$.
  - Elliptic: $DD'' < 0$.
  - Exceptional: $D'' = 0$.

*3.2.5. Small time classification of extremals. Construction of semi-normal forms*

In this section, we present the basic results and techniques from singularity theory initiated in [16, 22] to analyze small time extremals curves, which will be the basic tool to analyze the optimal control problem. It is the construction of semi-normal form using the action of the pseudo-group of diffeomorphisms or symplectomorphisms, combined with specific feedback transformations.

*Classification of regular extremals.*
**Notations:** we denote by $\sigma_+$ (resp. $\sigma_-$) a bang arc with constant control $u = +1$ (resp. $-1$) and $\sigma_s$ is the singular arc. We denote $\sigma_1\sigma_2$ an arc $\sigma_1$ followed by $\sigma_2$. The surface $\Sigma : p \cdot G(q) = 0$ is called *switching surface* and let $\Sigma' \subset \Sigma$ given by: $p \cdot G(q) = p \cdot [G, F](q) = 0$. If $z(t) = (q(t), p(t))$ is an extremal curve on $[0, t_f]$, we note $\Phi(t) = p(t) \cdot G(q(t))$ the *switching function* (which codes the switching times). Differentiating twice with respect to time one gets:

$$\dot{\Phi}(t) = p(t) \cdot [G, F](q(t))\,, \tag{26}$$

$$\ddot{\Phi}(t) = p(t) \cdot ([[G, F], F](q(t)) + u(t)\,[[G, F], G](q(t))). \tag{27}$$

From this calculus we deduce.

*Ordinary switching time.* A time $t \in ]0, t_f[$ is called an *ordinary* switching time and $z(t) \in \Sigma$ an ordinary switching point if $\Phi(t) = 0$ and $\dot\Phi(t) \neq 0$. Clearly we have.

**Lemma 5.** *In the ordinary case, near $z(t)$ every extremal solution projects onto $\sigma_+\sigma_-$ if $\dot\Phi < 0$ and $\sigma_-\sigma_+$ if $\dot\Phi > 0$.*

*Fold case.* If $\Phi(t) = \dot\Phi(t) = 0$, then $z(t) \in \Sigma'$. The situation is more intricate and is technically complicated to analyze, see [22] for the details. Let $u = \varepsilon$, $\varepsilon = \pm 1$ and $\ddot\Phi_\varepsilon(t) = p(t) \cdot ([[G, F], F](q(t)) + \varepsilon[[G, F], G](q(t)))$. If $\ddot\Phi_\varepsilon(t) \neq 0$ for $\varepsilon = \pm 1$, the point $z(t)$ is called a *fold point* and we have three cases assuming $\Sigma'$ is a regular surface of codimension two.

**Case 1:** *parabolic case*: $\ddot\Phi_+(t)\ddot\Phi_-(t) > 0$.

**Case 2:** *hyperbolic case*: $\ddot\Phi_+(t) > 0$ and $\ddot\Phi_-(t) < 0$.

**Case 3:** *elliptic case*: $\ddot\Phi_+(t) < 0$ and $\ddot\Phi_-(t) > 0$.

Denote by $u_s(t)$ the singular control given by

$$p(t) \cdot ([[G, F], F](q(t)) + u_s(t)[[G, F], G](q(t))) = 0.$$

From the above classification, we deduce. In the hyperbolic or elliptic case, through $z(t)$ if $p(t) \cdot [[G, F], G](q(t)) \neq 0$ there exists a singular extremal which is strictly admissible that is $|u_s(t)| < 1$. Moreover we are in the hyperbolic case (resp. elliptic) if this quantity is $> 0$ (resp. $< 0$). In the parabolic case, it can be absent (for instance in the linear case: $F(q) = A\,q$, $G(q) = b$) or not admissible that is $|u_s(t)| > 1$.
One has

**Theorem 4.** *In the neighborhood of $z(t)$ every extremal projects onto:*

- *In the parabolic case: $\sigma_+\sigma_-\sigma_+$ or $\sigma_-\sigma_+\sigma_-$.*
- *In the hyperbolic case: $\sigma_\pm\sigma_s\sigma_\pm$.*
- *In the elliptic case: every extremal is bang-bang, i.e. of the form $\sigma_+\sigma_-\ \sigma_+\sigma_- \ldots$ but the number of switches is not uniformly bounded.*

Note that the elliptic case opens the road to the so-called *Fuller phenomenon* [23, 18] where a connection with a singular arc can be realized but with an infinite number of switches.

The general tool to analyze this situation is the concept of semi-normal form and we shall make a simplified presentation using the planar case. Also this will lead to extensions which will be crucial in our next section of classifications of extremals near a manifold of codimension one.

*Introducing semi-normal forms.* We consider a 2D-system: $\dot q = F(q) + u\,G(q)$, $q = (x, y)$. We note $C$ : $\det(F, G) = 0$ the *collinearity set* and we restrict our system to $U$ : $\mathbb{R}^2 \setminus C$. Using the previous computations, singular trajectories are located on $S$ : $\det(G, [G, F]) = 0$. The direction of the adjoint vector $p$ is obtained with $p \cdot G = 0$ and using the previous notation the singular control is $u_s = -D'/D$. One picks a reference singular curve $\sigma_s(t)$. In a $C^0$-neighborhood of this curve we can choose coordinates $q = (x, y)$ such that: $\sigma$ : $t \to (t, 0)$ and $G = \frac{\partial}{\partial y}$. This leads to the following semi-normal form:

$$\dot x = 1 + \varepsilon y^2 + \ldots, \quad \dot y = (u - u_s(x)) + \ldots,$$

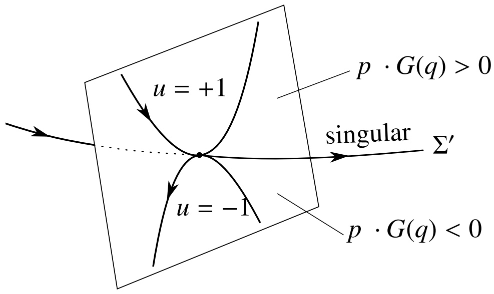


Figure 2: Fold case in the hyperbolic case in dimension 2 and the turnpike phenomenon

where the terms ... are not relevant in our study. Note if we relax the bound $|u| \leq 1$, we get the limit problem so that $u_s(x)$ can be set to 0 using a feedback transformation.

Clearly the optimality status of the reference singular arc can be immediately deduced from this form. If $\varepsilon < 0$, we are in the hyperbolic case and the singular direction is time minimizing in a $C^0$-neighborhood of the reference singular extremal and time minimizing in the elliptic case. The adjoint vector is oriented with the convention $p \cdot F > 0$ and we deduce the standard *turnpike phenomenon* characteristic of the hyperbolic situation, that is, provided $|u_s| \leq 1$, the optimal policy is of the form $\sigma_\pm\sigma_s\sigma_\pm$. (Note it is valid not only for small time). It is represented on Fig.2 in the $(q, p)$ space. Of course, this situation doesn't cover the various situations encountered in the applications. One important case being the saturation phenomenon where $|u_s| = 1$, which will be discussed later.

Next we shall introduce the *bridge phenomenon*.

*Connecting singular arcs: the bridge phenomenon.* The aim of this paragraph is to analyze the connection between singular extremals, extending the previous classification. For the sake of the tutorial aspect we shall use a planar semi-normal form.

**Definition 4.** *A bridge is a bang arc $\sigma^b$ connecting two singular arcs $\sigma_s^1$, $\sigma_s^2$ so that $\sigma_s^1\sigma^b\sigma_s^2$ is an admissible extremal curve.*

*Birth of the model.* We consider the (limit) model:

$$\dot{x} = u, \quad \dot{y} = 1 - x^2y$$

so that $\sigma$ : $(0, t)$ is a singular arc which is hyperbolic if $y > 0$ and elliptic if $y < 0$. Using the notation $\dot{q} = F + uG$, singular trajectories are located on $S$ : $\det(G, [G, F])(q) = 0 = \{xy = 0\}$. Hence we have a ramification at $(0, 0)$ between two singular lines: the vertical axis which can be followed with the control $u_s = 0$ and the horizontal axis which can be followed by the "$u = \infty$" control.

To get our model we must bend this axis to make it tractable with a singular control $u_s \to \infty$ when going to 0. This leads to the following.

*The (symmetric) bridge model.* One takes

$$F = (1 - x^2y)\frac{\partial}{\partial y}, \quad G = -(y - 1)\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}. \tag{28}$$

The solutions of $G$ are circles contained on $(0,1)$, note a parameter $\lambda$ can be introduced using $1 \to \lambda$. Also one takes the bound $|u| \leq 1$, but an additional parameter is $|u| \leq M$. Lie brackets computations give us.

**Lemma 6.** *The singular set* $S$ : $\{q;\ \det(G,[G,F])(q) = 0\}$ *is the union of the vertical axis* $(Oy)$ *and the algebraic curve defined by:* $l(x,y) = x^2(1-2y) + 2y^3 - 4y^2 + 2y + 1 = 0$.

The equation $l(x,y) = 0$ is equivalent to $x = \pm\frac{\sqrt{2y^3-4y^2+2y+1}}{2y-1}$. The intersection with the vertical axis $x = 0$ is $(O, y_0)$, $y_0 \simeq -0.297157$.

We represent on Fig.3 the two singular trajectories: the set $l = 0$ denoted $\mathcal{L}$ and the vertical axis $(Oy)$ denoted $\mathcal{L}'$.

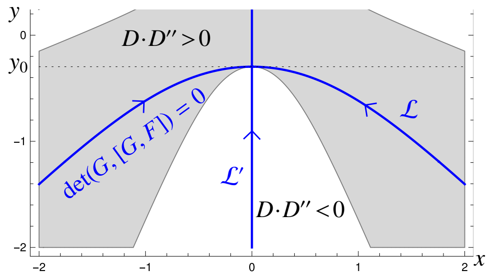


Figure 3: $(Oy)$ and $\mathcal{L}$ are two singular trajectories for the system (28) represented by two continuous lines. The filled regions are the points where $D \cdot D'' > 0$.

Further computations lead to.

**Proposition 3.** *The vertical singular line* $\mathcal{L}'$ *is hyperbolic for* $y > y_0$ *and elliptic for* $y < y_0$. *The singular line* $\mathcal{L}$ *is hyperbolic and the singular control along* $\mathcal{L} \cap \{x \leq 0\}$ *is given by:*

$$u_s(q) = -\frac{D'(q)}{D(q)} = \frac{A}{B}$$

*where* $A = -8y^7 + 30y^6 - 44y^5 + 38y^4 - 27y^3 + 15y^2 - 6y + 2$ *and* $B = \sqrt{(2y-1)(2y^3-4y^2+2y+1)}\left(8y^3 - 15y^2 + 9y - 3\right)$.

We represent on Fig.4 this singular control showing in particular the existence of two saturating points $|u| = 1$.

To conclude, this leads to construct a bridge using a simple numeric simulation, see Fig.5, and an extremal solution which projects onto $\sigma_-\sigma_{\mathcal{L}}\sigma_+^b\sigma_{\mathcal{L}'}$, see Fig.6.

Note that time minimality can be analyzed using standard discussion, moreover mathematical estimates can be obtained near $(O, y_0)$, making $\lambda \to +\infty$ and $M \to +\infty$, see Fig.7 for the effect of $\lambda \to +\infty$ so that $y_0 \to 0$ and $\mathcal{L}$ tends to the horizontal axis.

**Remark 4** (Geometric remark)**.** *Interaction between the two singular curves is coded by the singularities of the flow* $\dot{q} = F(q) - \frac{D'(q)}{D(q)}G(q)$ *since* $D' + u_s D = 0$. *It can be analyzed using a time reparametrization using the dynamics:* $\dot{q} = D(q)F(q) - D'(q)G(q)$, *with singular equilibrium in* $D = D' = 0$. *This geometric remark is crucial for the extension to the non planar case.*

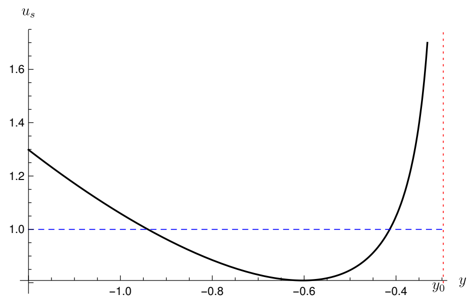


Figure 4: Singular control $u_s$ for $x < 0$. There exists two saturating points.

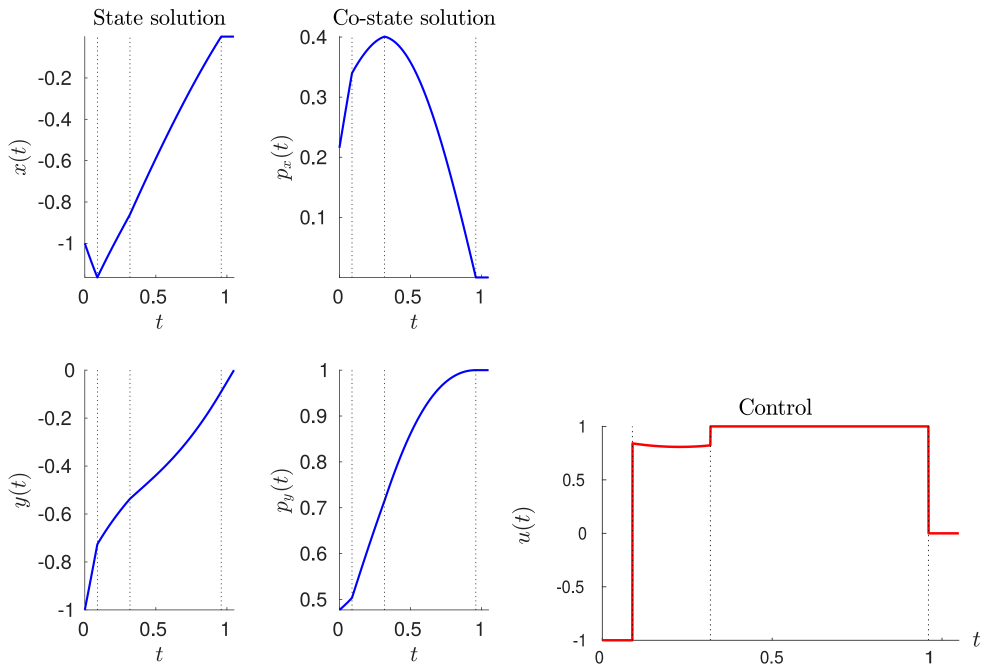


Figure 5: Time evolution of an extremal for the problem (28) of reaching the origin in minimal time starting from $(x(0), y(0)) = (-1, -1)$.

## 4. Time minimal synthesis near the terminal manifold

The basic technical study applicable to chemical batch reactions was developed in the series of papers [7, 11, 10, 9, 24]. The problem is the following. Consider the system: $\dot{q} = F(q) + u\,G(q)$, $|u| \leq 1$ with terminal manifold $N = f^{-1}(0)$ where $f : \mathbb{R}^n \to \mathbb{R}$ is a submersion. One consider the following *local problem*: take $q_0 \in N$, compute, in a small neighborhood $U$ of $q_0$ (the size of $U$ is not a priori known), the optimal closed control $u^*(q)$ to steer (staying in $U$) from $q \in N$ to $N \cap U$, in minimum time. Such a problem is called the local time minimal synthesis, with terminal manifold. Note that a lot of central work in this area was done in the $80's$, see [31, 25, 13] when the terminal manifold is a point, to classify in small dimension the optimal synthesis in

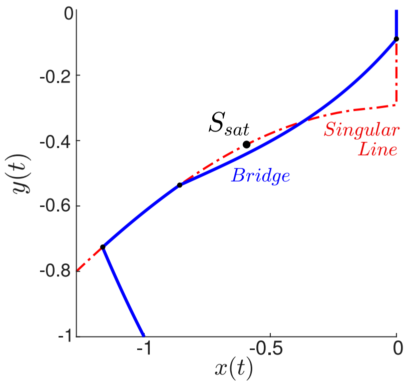


Figure 6: Trajectory associated to the extremal of Fig.5. $\sigma_+^b$ is a bridge connecting two switching points of the singular set and the singular control saturates at the point $S_{sat}$.

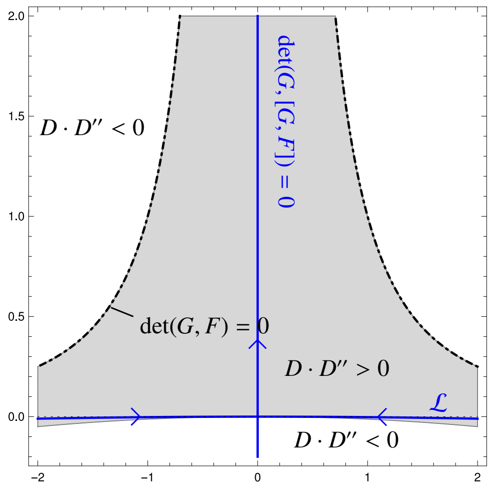


Figure 7: $(Oy)$ and $\mathcal{L}$ corresponding singular trajectories for the system (28) where $G$ is replaced by $G = -(y-\lambda)\,\frac{\partial}{\partial x} + x\,\frac{\partial}{\partial y}$ and $\lambda = 200$. The dash-dotted curve corresponds to the collinearity set. The filled regions are the points where $D{\cdot}D'' > 0$.

relation with the Lie algebraic structure of $(F, G)$ at the given point $q_0$. If all those contributions are valuable in our study, we shall make the computation explicit in the case where the terminal manifold $N:\ f = 0$ is of *codimension one* and using also different tools, that is the construction of *semi-normal forms* for the action of the pseudo-group $G$ formed by local diffeomorphism and feedback transformation $u \to -u$ (so that $\sigma_+$ and $\sigma_-$ can be exchanged). This technique is coming from singularity theory, see [26] for a useful introduction of this area. Note we shall work in the $C^k$−category, where $k \geq 1$ will not be precised and the semi-normal form is related to a semi-algebraic stratification on the jets spaces of $(F, G, N)$. One needs to introduce some definitions and concepts.

### 4.1. Notations and definitions

Note that for chemical systems $N: \ c_1 = d$ and the chemical species are such that $c_1(0) < d$. Define $N^\perp = \{(q,p);\ p \cdot v = 0, \forall v \in T_qN\}$ and let $n$ be the normal to $N$ oriented as the outward normal to $N$ (using the chemical model). Let $z = (q,p)$ be a BC-extremal, $t \in [t_f, 0]$, $t_f < 0$ (since we integrate backwards from the terminal manifold). A time $s$ is called *switching time* if $s$ belongs to the closure of the switching time on $[t_f, 0]$ (in the general setting, switches can accumulate due to the *Fuller phenomenon* [23]). We shall denote by $K$ the switching points and by $W$ the set of switching points for minimizing curves. If $W$ is stratified, a stratum is of the *first kind* if the optimal trajectories are tangent and of the *second kind* if they are transverse. The *splitting locus* $L$ is the set of points where the optimal control is not unique and the *cut locus* $C$ is the closure of the set of points where the optimal trajectory loses its optimality. The reader can refer to [3], [14] and [31] for the details and results about the concepts in the frame of *semi-analytic geometry*.

Next one needs concepts from singularity theory.

*Concepts and definitions.* $F, G$ and $N$ are in the $C^w$-category, $N = f^{-1}(0)$, $f$ is a submersion. The set of triplet $(F, G, f)$ is endowed with $C^\infty$-Whitney topology. We denote by $j^kF(q_0)$ (resp. $j^kG(q_0)$, $j^kf(q_0)$) the *k-jet* of $F$ (resp. $G$, $f$) that is the Taylor expansion at order $k$. We say that the system $(G, F, f)$ has at $q_0$ a singularity of codimension $i$ if $j^kF(q_0),\ j^kG(q_0),\ j^kf(q_0) \in \Sigma_i$, where $\Sigma_i$ is a semi-algebraic submanifold of codimension $i$ in the jet space.

Taking a point $q_0$ with a singularity of codimension $i$, an *unfolding* is a $C^0$-change of coordinates $\phi$ near $q_0$ such that (small) time minimal synthesis is described by a system $\dot{\bar{x}} = F(\bar{x}, \lambda) + u\, G(\bar{x}, \lambda)$, $|u| \le 1$, $\bar{x} \in \mathbb{R}^{n-m}$ and $\lambda$ is a parameter.

### 4.2. Local syntheses

We shall present the main step to compute the time minimal synthesis and thanks to the concept of unfoldings we shall restrict our study to the 3-dimensional case, which is also the situation corresponding to our test bed cases. The system is written $\dot{q} = F(q) + u\, G(q)$, $|u| \le 1$ and let $q = (x, y, z)$ be the coordinates. The terminal manifold is $N$ and we suppose that the problem is *flat* that is $G$ being identified to $\frac{\partial}{\partial z}$ and $G$ is tangent everywhere to $N$. If $n$ is normal to $N$, outwardly oriented, we introduce the following to *stratify* the terminal manifold.

- $\mathcal{S}$: singular locus defined by $\{q \in N;\ n \cdot [G, F](q) = 0\}$,
- $\mathcal{E}$: exceptional locus defined by $\{q \in N;\ n \cdot F(q) = 0\}$.

Note that since the problem is flat: $n \cdot G(q) = 0$ if $q \in N$, that is $N^\perp \subset \Sigma$ : switching surface.

#### 4.2.1. Generic case

Take $q_0 \in N$, $q_0 \notin \mathcal{S}$, $q_0 \notin \mathcal{E}$, then $(n, q_0)$ is an ordinary switching point and according to section 3.2.5, near $q_0$ every $BC$-extremal is of the form $\sigma_+$ if $n \cdot [G, F](q_0) < 0$ and of the form $\sigma_-$ if $n \cdot [G, F](q_0) > 0$. This gives the local synthesis.

#### 4.2.2. Generic hyperbolic singular case

One can take $q_0 = 0$ and we make the following assumptions at 0.

- The tangent space to $N$ at 0 is $G(0)$, $[G, F](0)$.

- The set of points $L$ where $[G, F]$ is tangent to $N$ is a simple curve passing through 0 and transverse to $G$.
- $D(0)$ and $D''(0)$ are non zero.

With those assumptions, through 0, there exists a single $BC$-extremal denoted $\hat{\sigma}$ transverse to $N$. Near 0 one can make the following normalization (that is using adapted coordinates): $G$ being identified to $\frac{\partial}{\partial z}$, $L$ to the axis $(Oy)$ and $\hat{\sigma}$ can be identified to: $t \to (t, 0, 0)$ with image being the $(Ox)$-axis. Note that the target is identified to $x = 0$. The system is written as:

$$\begin{aligned}
\dot{x} &= 1 + \sum_{i+j>0} a_{ij}(x) y^i z^j \\
\dot{y} &= \sum_{i+j>0} b_{ij}(x) y^i z^j \\
\dot{z} &= (u - \hat{u}(x)) + \sum_{i+j>0} c_{ij}(x) y^i z^j
\end{aligned}$$

where $\hat{u}(x)$ is the singular control associated to $\hat{\sigma}$. One further normalization leads to take $[G, F]_{|\hat{\sigma}} = [G, F](0)$. Here we obtain a semi-normal form:

$$\begin{aligned}
\dot{x} &= 1 + a(x)z^2 + 2b(x)yz + c(x)y^2 + \varepsilon_1 \\
\dot{y} &= d(x)y + e(0)z + \varepsilon_2 \\
\dot{z} &= (u - \hat{u}(x)) + f(x)y + g(0)z + \varepsilon_3
\end{aligned}$$

with $b(0) = 0,\ e(0) \neq 0$ and $\varepsilon_1$ (resp. $\varepsilon_2,\ \varepsilon_3$) are terms of order $\geq 3$ (resp. $\geq 2$) in $y, z$.

Computing, one has $n \cdot [[F, G], G](0) = 2a(0)$. We assume:

- $a(0) < 0$ (hence the singular arc is hyperbolic) and moreover $\hat{u}(0) \in ]-1, +1[$ that is the singular arc is strictly admissible.

Hence $(q_0, n)$ is an *hyperbolic fold point* and using 3.2.5 an extremal near such a point is $\sigma_\pm \sigma_s \sigma_\pm$. Moreover arcs $\sigma_+$ and $\sigma_-$ are defined on $[t_f, 0]$ such that $\sigma_+(0),\ \sigma_-(0)$ near $q_0$ are $\sigma_+$ in the domain $z < 0$ and $\sigma_-$ in the domain $z > 0$ and are not intersecting since $\dot{z} \sim (u - \hat{u}(0))$, hence: $z(t) = (\varepsilon - \hat{u}(0))\, t + s$, $s = z(0)$ and $\varepsilon = \pm 1$. Using the normalization, one can evaluate the switches of $BC$-arc $\sigma_+$ and $\sigma_-$ for $t < 0$. One has:

$$\begin{aligned}
&p_1(t) = 1 + o(1),\ \ p_2(t) = o(1), \\
&\dot{p}_3(t) \sim -2a(0)p_1 + (\varepsilon - \hat{u}(0))\, z + \dots .
\end{aligned} \tag{29}$$

Hence, we have $p_3(t) \sim -2a(0)\, t\ (s + (\varepsilon - \hat{u}(0))\, t/2 + o(s, t))$. Using $\varepsilon s < 0$, one gets that $p_3(t)$ is not vanishing for $t < 0$. Hence we deduce the following which gives the $C^0$-unfolding.

**Proposition 4.** *Under arc assumptions near* 0*, the optimal synthesis is described by the model:* $\dot{x} = 1 + a(0)z^2$, $\dot{y} = 0$, $\dot{z} = (u - \hat{u}(0))$ *and is represented in each invariant plane* $y =$ *constant by Fig.8.*

Assume now that $\hat{u}(0) \notin ]-1, +1[$ then $P = (q_0, n)$ is a *parabolic fold* point and the synthesis can be again deduced from our normalizations. Each extremal is bang-bang with at most two switchings, and one is located at the terminal point on $N$.

Using the previous estimates one can compute the optimal switching locus $W_-$ near $N$ and the optimal synthesis is represented on Fig.9 in an invariant plane $y =$ constant.

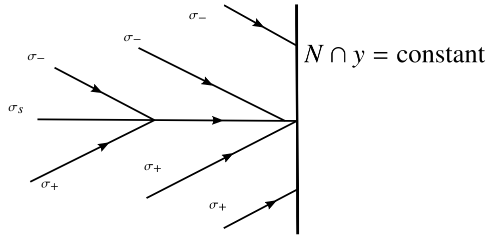


Figure 8: Hyperbolic case. $|\hat{u}(0)| < 1$.

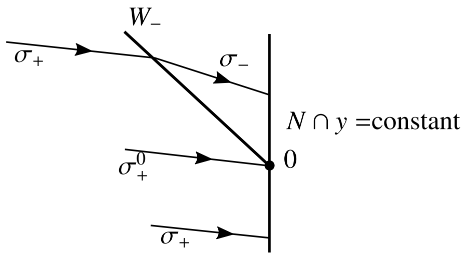


Figure 9: Parabolic case: $\hat{u}(0) \notin ]-1, 1[$.

*Saturate case.* One shall briefly present the transition between the hyperbolic and parabolic case due to the saturation of the control $|\hat{u}(0)| = 1$, see [10] for a complete study. From our previous analysis the model is:

$$\begin{aligned}
\dot{x} &= 1 + a(x)z^2 + 2b(x)yz + c(x)y^2 \\
\dot{y} &= d(x)y + c(0)z \\
\dot{z} &= (u-1) - \hat{u}_x x - \hat{u}_y y
\end{aligned}$$

with $a(0) < 0$, $b \neq 0$ and $\hat{u}_x = \frac{\partial \hat{u}}{\partial x}(0)$, $\hat{u}_y = \frac{\partial \hat{u}}{\partial y}(0)$ and $\hat{u}_x,\ \hat{u}_y$ are generically non zero and we may assume $\hat{u}_y > 0$. Computations lead to the two cases represented in Figs.10-11.

Note that the existence of two syntheses is discriminated by vanishing (case 2) and the vanishing (case 1) of the singular curve.

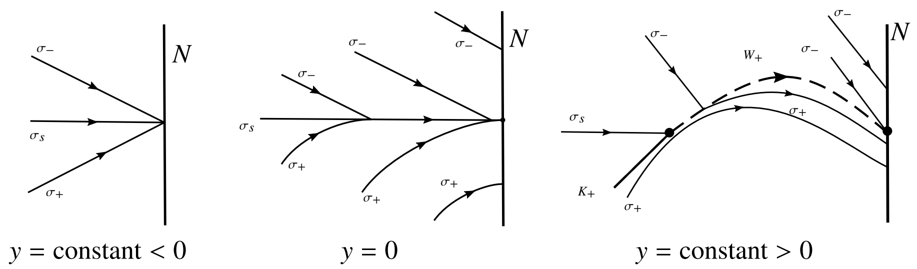


Figure 10: *Saturation case:* Case 1: $\hat{u}_x(0) > 0$.

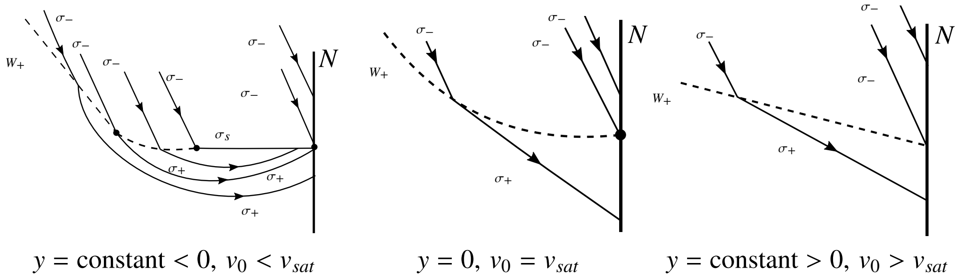


Figure 11: *Saturation case:* Case 2: $\hat{u}_x(0) < 0$.

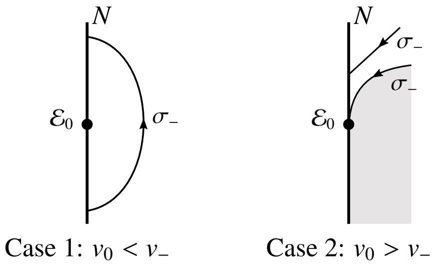


Figure 12: Local synthesis near $\mathcal{E}_0 = \mathcal{E} \cap (v = v_0)$ in the leaf $v = v_0$ when $\alpha > 1$.

*4.2.3. The exceptional case*

The exceptional case corresponds either to bad controllability properties of the system, related to singular arcs or bad accessibility property of the target. We made a concise presentation related to our study for chemical systems, see [24] for the details.

*The generic case.* It is a situation with (minimal) contact one of bang arcs with the target manifold. In this case, restricting to a planar case thanks to the concept of unfoldings we have two cases represented on Fig.12 obtained by obvious topological analysis. We note $\mathcal{E}_0$ the point where arcs $\sigma_+$, $\sigma_-$ are tangent. In the case 2, the black domain represents the set of the domain with no optimal trajectory.

*The codimension one case.* The situation is more intricate, since we cannot use a planar invariant foliation. We have several cases corresponding to two situations.

**Situation 1.** Bang arc with a contact of *order two* with the target at a point of $\mathcal{E}$. We have two cases represented on Fig.13-14.

**Situation 2.** It concerns $\mathcal{E} \cap \mathcal{S}$ which is a singular arc tangent to $N$ and according to our classification it concerns a singular exceptional arc. This complicated case is discussed in [24].

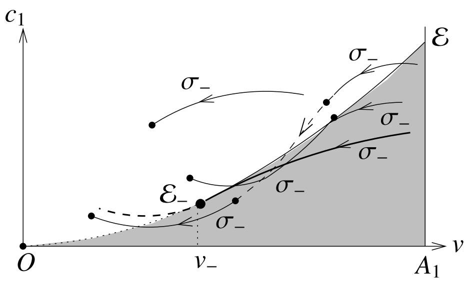


Figure 13: **Contact order** 2. Non accessible points: grey region, $\mathcal{E}_-$: accessible. Local synthesis near $\mathcal{E}_-$.

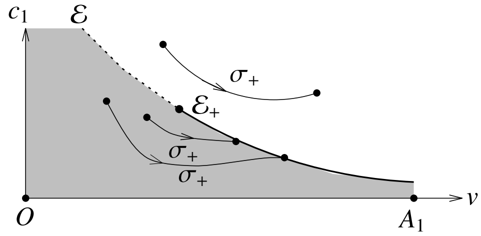


Figure 14: **Contact order** 2. Non accessible points: grey region, $\mathcal{E}_+$: non accessible. Local synthesis near $\mathcal{E}_+$.

## 5. Application to the two test bed cases

*5.1. The case* $A \xrightarrow{k_1} B \xrightarrow{k_2} C$

The system $\dot{q} = F(q) + u\,G(q)$, using the coordinates $q = (x, c_2, v)$, $x = \ln c_1$ takes the form

$$\begin{aligned} \dot{x} &= -v \\ \dot{c}_2 &= ve^x - \beta v^\alpha c_2 \\ \dot{v} &= u \end{aligned} \tag{30}$$

and in the coordinates $q = (x, y, v)$ $y = c_2/c_1$ one gets

$$\begin{aligned} \dot{x} &= -v \\ \dot{y} &= v - \beta v^\alpha y + vy \\ \dot{v} &= u. \end{aligned} \tag{31}$$

It is integrated on $[t_f, 0]$ together with the adjoint equation:

$$\dot{p} = -p\left(\frac{\partial F}{\partial q}(q) + u\,\frac{\partial G}{\partial q}(q)\right).$$

Without losing any generality one may assume $|u| \leq 1$.

*5.1.1. Lie brackets computations*

One uses the coordinates $q = (x, y, v)$ and we get:

$F(q) = -v\,\frac{\partial}{\partial x} + (v - \beta v^\alpha y + vy)\frac{\partial}{\partial y}\,, \quad G(q) = \frac{\partial}{\partial v}\,,$
$[G, F](q) = \frac{\partial}{\partial x} + (-1 + \alpha\beta v^{\alpha-1} y - y)\,\frac{\partial}{\partial y}\,,$
$[[G, F]\,, F]\,(q) = (\alpha - 1)\beta v^\alpha\,\frac{\partial}{\partial y}\,,$
$[[G, F]\,, G]\,(q) = \alpha(\alpha - 1)\beta v^{\alpha-2} y\frac{\partial}{\partial y}.$

*5.1.2. Singular arcs*

Recall

$$D(q) = \det(G(q), [G,F](q), [[G,F],G](q)),$$
$$D'(q) = \det(G(q), [G,F](q), [[G,F],F](q)), \quad (32)$$
$$D''(q) = \det(G(q), [G,F](q), F(q)).$$

and the singular control is defined by: $D'(q) + u_s(q)\,D(q) = 0$.

Hence,

**Lemma 7.** *We have $D(q) = \alpha(\alpha-1)\beta v^{\alpha-2}y$, $D'(q) = (\alpha-1)\beta v^{\alpha}$, $D''(q) = (\alpha-1)\beta v^{\alpha}y$, so that,*

1) *The singular control is given by $u_s = -v^2/(\alpha y)$ and is negative. Moreover $v$ decreases along a singular arc. The singular control saturates at $S$ : $v^2/(\alpha y) = 1$*

2) *The singular trajectories are hyperbolic.*

One needs also

**Lemma 8.** *Let $z(\cdot) = (q(\cdot), p(\cdot))$ be a BC-extremal on $[t_f, 0]$ in the coordinates $q = (x, c_2, 0)$ so that $p(0) = (0,1,0)$. Then at any $t < 0$ one has $p_1(t) > 0$ and $p_2(t) > 0$.*

*Proof.* The adjoint equation gives

$$\dot{p}_1 = -p_2 v e^x, \quad \dot{p}_2 = p_2\beta v^{\alpha}$$

and the result follows. □

**Lemma 9.** *Along a BC-singular extremal one has with $\alpha > 1$, $\dot{c}_2 > 0$ and $c_2$ increases.*

*Proof.* From Lemma 8, in the coordinates $q = (x, c_2, 0)$, one has $p_1(t) > 0$ and $p_2(t) > 0$ for any $t < 0$ and eventually $p_1(0) = 0$, $p_2(0) = 1$. Using $p \cdot [G,F](q) = 0$ we get the relation:

$$p_1 = p_2(c_1 - \alpha\beta v^{\alpha-1}c_2)$$

and for $t < 0$, $p_1 > 0$, $p_2 > 0$, hence we obtain

$$c_1 - \alpha\beta v^{\alpha-1}c_2 > 0 \quad (33)$$

and we have

$$\dot{c}_2 = v(c_1 - \beta v^{\alpha-1}c_2). \quad (34)$$

Since $\alpha > 1$, (33) implies that the right member of (34) is positive. The result is also true at the final time if (eventually) $c_2$ belongs to $c_2 = d$ since the intersection $\mathcal{E}\cap\mathcal{S} = \emptyset$ with $\mathcal{E} : n\cdot F(q) = 0$, $\mathcal{S} : n \cdot [G,F](q) = 0$. □

*5.1.3. Properties of the switching function*

In this section we use the coordinates $q = (x, y, v)$ and we consider the switching function: $\Phi(t) = p(t)\cdot G(q(t))$ along an extremal $z(\cdot) = (q(\cdot), p(\cdot))$ on $[t_f, 0]$. Computing one has:

**Lemma 10.** *If $z(\cdot)$ is smooth, one has $\ddot{\Phi}(t) = p_2(t)(\alpha-1)\beta v^{\alpha-2}\left(v^2 + u\alpha y\right)$. If $z(\cdot)$ is a BC-extremal, $p_2(t) > 0$ on $[t_f, 0]$. Hence if $u = +1$, $\Phi(t)$ is strictly convex (resp. concave) if $\alpha > 1$ (resp. $\alpha < 1$).*

**Corollary 1.** *If $\sigma_+$ is BC arc on $[t_1, t_2]$ and if $t_2$ is a switching time then $t_1$ cannot be a switching time if $\alpha > 1$.*

*Proof.* Assume $t_1, t_2$ be switching times. Then one must have

$$\dot{\Phi}(t_1) \geq 0 \text{ and } \dot{\Phi}(t_2) \leq 0.$$

A contradiction since $\ddot{\Phi}(t) > 0$ from Lemma 10. □

**Lemma 11.** *Let $\sigma_-$ be an extremal on $[t_2, t_3]$. Assume $\dot{y}(t_2) > 0$ then $\dot{y}(t) > 0$ for $t \geq t_2$, assuming $\alpha > 1$.*

*Proof.* One has:

$$\dot{y} = v\left(1 - \beta v^{\alpha-1} y + y\right)$$

and assume there exists $\tau'$, $\dot{y}(t) > 0$ for $t < \tau'$, $\dot{y}(\tau') = 0$ and $\dot{y}(\tau) < 0$ for $[\tau', \tau]$. Differentiating and evaluating at $\tau'$ one has

$$\ddot{y}(\tau') = v\left(-(\alpha - 1)\beta y v^{\alpha-2}\dot{v} + 1\right)$$

with $\dot{v} = -1$ along $\sigma_-$. Hence since $\alpha > 1$, $\ddot{y}(\tau') > 0$. A contradiction. □

**Lemma 12.** *A sequence $\sigma_s\sigma_-$ with non empty subarc cannot exist for a BC-extremal if $\alpha > 1$.*

*Proof.* Assume such a sequence exists with $\sigma_s$ on $[t_1, t_2]$ and $\sigma_-$ on $[t_2, t_3]$. One has the relations:

$$\Phi(t_2) = \dot{\Phi}(t_2) = 0, \quad \Phi(t_3) = 0.$$

Since $\Phi(t_2) = \Phi(t_3) = 0$, from Rolle's theorem, there exists $t_2 < t_2' < t_3$ such that $\dot{\Phi}(t_2') = 0$.

Using Rolle's theorem again with $\dot{\Phi}(t_2) = \dot{\Phi}(t_2')$, there exists $t_2 < t_2'' < t_2'$ such that $\ddot{\Phi}(t_2'') = 0$.

Note that from Lemma 7 and Lemma 10 one has along $\sigma_-$:

$$\ddot{\Phi}(t) = \frac{p_2(t)(\alpha - 1)\beta v^{\alpha-2}}{\alpha y}(-1 - u_s)$$

with $u_s = -v^2/(\alpha y)$.

Hence if $\ddot{\Phi}(t_2'') = 0$ one has $u_s(t_2'') = -1$ and $\sigma_-$ meets the saturating set $S : u_s = -1$.

At the junction time $t_2$ between $\sigma_s$ and $\sigma_-$, one has $u_s(t_2) \geq -1$, $\dot{c}_2(t_2) > 0$ from Lemma 9 and along $\sigma_- : \dot{y} = \dot{c}_2/c_1 + c_2/c_1\, v \geq 0$ and $\dot{v} < 0$.

Moreover along $\sigma_-$, sign $\ddot{\Phi}(t) =$ sign $(-1 - u_s)$, since $\dot{y} \geq 0$, $\dot{v} \leq 0$, $-1 - u_s$ is a decreasing function of time.

Since $\ddot{\Phi}(t_2) \leq 0$ it turns out that for $t \in ]t_2, t_3[$ one has $\ddot{\Phi}(t_2) < 0$.

This contradicts $\ddot{\Phi}(t_2'') > 0$ for $t_2'' > t_2$. □

From Corollary 1 and Lemma 12 we deduce.

**Theorem 5** ($\alpha > 1$)**.** *Every optimal trajectory has at most two swtichings and is of the form $\sigma_+\sigma_-\sigma_s$ where each arc of the sequence can be empty.*

*5.1.4. Local optimal synthesis near N, the case $\alpha < 1$*

It will be easily follows from the classification of Section 4.1. We represent on Fig.15 the stratification of the terminal manifold by $\mathcal{S} : n \cdot [G, F](q) = 0$ and $\mathcal{E} : n \cdot F(q) = 0$.

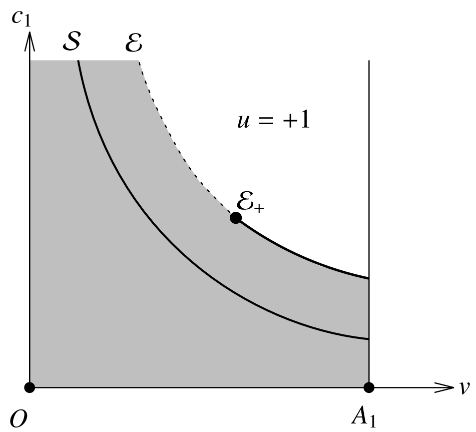


Figure 15: Stratification of the terminal manifold $N$ for $\alpha < 1$. Non-accessible points are in the filled region and on the dotted-line of $\mathcal{E}$.

The optimal policy near $N$ is $\sigma_+$.

**Theorem 6.** *In the case $\alpha < 1$, the local optimal policy is $\sigma_+$.*

*5.1.5. Local optimal synthesis near N, the case $\alpha > 1$*

Again we use the classification of Section 4.1 but the situation is more intricate. It is represented on Fig.16 and we refer to Section 4.1 for the corresponding figures.

- Singular hyperbolic arcs reaching the manifold are on $\mathcal{S}$ and we have a saturating point where $u_s = -1$.
- The boundary of the accessibility set is associated to $\mathcal{E}$, with $\mathcal{E}_-$ accessible.

The global optimal policy follows from Theorem 5: an optimal trajectory being of the form $\sigma_+\sigma_-\sigma_s$ where each arc of the sequence can be empty. It can be numerically obtained, integrating backwards on $[t_f, 0]$ using the local synthesis resolution of our analysis.

- Near a point $\mathcal{E}_0 \neq \mathcal{E}_-$ of $\mathcal{E}$, the optimal synthesis is described by a $C^0$ invariant foliation $\mathcal{F} : (v = v_0)$ the leaves of which are given by Fig.12; near $\mathcal{E}_-$ there is no such foliation and the synthesis is given by Fig.13.
- Near the point $S_{\text{sat}}$ of $\mathcal{S}$, the optimal synthesis is given by Fig.11.

*5.2. The McKeithan scheme and the computational complexity*

Recall that the network is
$$\begin{tikzcd} T+M \arrow[r, "k_1"] & A \arrow[r, "k_2"] \arrow[l, bend left, "k_3"] & B \arrow[ll, bend left, "k_4"] \end{tikzcd}$$
and the system $\dot{q} = F(q) + u\,G(q)$, using the coordinates $q = (x, y, v)$, $x = [A]$, $y = [B]$, $v = k_1$ and reduced to the stoichiometric class

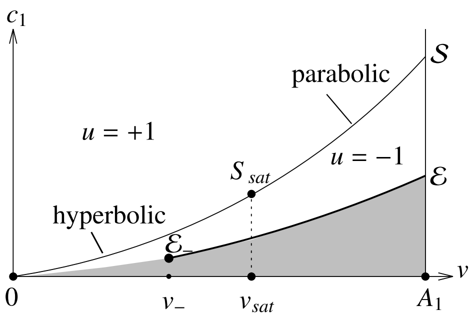


Figure 16: Stratification of the manifold $N$ for $\alpha > 1$. Non-accessible points are in the filled region and on the dotted-line of $\mathcal{E}$ and points on $\mathcal{E}_-$ are accessible.

$T + M + A = \delta_1$ and $T + M + B = \delta_2$ takes the form

$$\dot{x} = -\beta_2 x v^{\alpha_2} - \beta_3 x v^{\alpha_3} - \delta_3 v\,(x + y) + \delta_4 v + v\,(x + y)^2$$
$$\dot{y} = \beta_2 x v^{\alpha_2} - \beta_4 y v^{\alpha_4}$$

with $0 \leq x \leq \delta_1$, $0 \leq y \leq \delta_2$, $\delta_3 = \delta_1 + \delta_2$, $\delta_4 = \delta_1\,\delta_2$, $k_2 = \beta_2\,v^{\alpha_2}$, $k_3 = \beta_3\,v^{\alpha_3}$, $k_4 = \beta_4\,v^{\alpha_4}$.

*5.2.1. Lie brackets computations*

One gets:

- $F = \big(-\beta_2 x v^{\alpha_2} - \beta_3 x v^{\alpha_3} - \delta_3 v(x + y) + \delta_4 v + v\,(x + y)^2\big)\frac{\partial}{\partial x} + \big(\beta_2 x v^{\alpha_2} - \beta_4 y v^{\alpha_4}\big)\frac{\partial}{\partial y}$,
- $G = \frac{\partial}{\partial v}$,
- $[G, F] = \big(x(\alpha_2\beta_2 v^{\alpha_2-1} + \alpha_3\beta_3 v^{\alpha_3-1} + \delta_3) + \delta_3 y - \delta_4 - x^2 - 2xy - y^2\big)\frac{\partial}{\partial x} + \big(\alpha_4\beta_4 y v^{\alpha_4-1} - \alpha_2\beta_2 x v^{\alpha_2-1}\big)\frac{\partial}{\partial y}$,
- $[[G, F], G] = \big(x(\alpha_2\beta_2(\alpha_2-1)v^{\alpha_2-2} + \alpha_3\beta_3(\alpha_3-1)v^{\alpha_3-2})\big)\frac{\partial}{\partial x} + \big(y\alpha_4\beta_4(\alpha_4-1)v^{\alpha_4-2} - x\alpha_2\beta_2(\alpha_2-1)v^{\alpha_2-2}\big)\frac{\partial}{\partial y}$,
- $[[G, F]\,F] = \big(-xv^{\alpha_2}\beta_2\delta_3(\alpha_2 - 1) - yv^{\alpha_2}\beta_2\delta_3(\alpha_2 - 1) + v^{\alpha_2}(\alpha_2\beta_2\delta_4 + xy(2\alpha_2\beta_2 - 2\beta_2) - \beta_2\delta_4) + x^2(\alpha_2\beta_2 - \beta_2)v^{\alpha_2} + y^2(\alpha_2\beta_2 - \beta_2)v^{\alpha_2} + yv^{\alpha_3}(\beta_3\delta_3 - \alpha_3\beta_3\delta_3) + v^{\alpha_3}(\alpha_3\beta_3\delta_4 - \beta_3\delta_4) + x^2(\beta_3 - \alpha_3\beta_3)v^{\alpha_3} + y^2(\alpha_3\beta_3 - \beta_3)v^{\alpha_3} + yv^{\alpha_4}(\alpha_4\beta_4\delta_3 - \beta_4\delta_3) + xy(2\beta_4 - 2\alpha_4\beta_4)v^{\alpha_4} + y^2(2\beta_4 - 2\alpha_4\beta_4)v^{\alpha_4}\big)\frac{\partial}{\partial x} + \big(x(v^{\alpha_2+\alpha_3-1}(\alpha_2\beta_2\beta_3 - \alpha_3\beta_2\beta_3) + v^{\alpha_2+\alpha_4-1}(\alpha_4\beta_2\beta_4 - \alpha_2\beta_2\beta_4)) + xv^{\alpha_2}(\alpha_2\beta_2\delta_3 - \beta_2\delta_3) + yv^{\alpha_2}(\alpha_2\beta_2\delta_3 - \beta_2\delta_3) + v^{\alpha_2}(-\alpha_2\beta_2\delta_4 + xy(2\beta_2 - 2\alpha_2\beta_2) + \beta_2\delta_4) + x^2(\beta_2 - \alpha_2\beta_2)v^{\alpha_2} + y^2(\beta_2 - \alpha_2\beta_2)v^{\alpha_2}\big)\frac{\partial}{\partial y}$.

*5.2.2. Singular arcs*

One has:

- $D(q) = ((\alpha_4 - 1)\alpha_4\beta_4 y v^{\alpha_4-3} - (\alpha_2 - 1)\alpha_2\beta_2 x v^{\alpha_2-3})(\alpha_2\beta_2 x v^{\alpha_2} + \alpha_3\beta_3 x v^{\alpha_3} + \delta_3 v(x+y) - \delta_4 v - vx^2 - 2vxy - vy^2) + x(\alpha_2^2\beta_2 v^{\alpha_2} - \alpha_2\beta_2 v^{\alpha_2} + (\alpha_3 - 1)\alpha_3\beta_3 v^{\alpha_3})(\alpha_2\beta_2 x v^{\alpha_2-3} - \alpha_4\beta_4 y v^{\alpha_4-3})$,

- $D'(q) = \beta_2 v^{\alpha_2-2}(\alpha_2\beta_2 x v^{\alpha_2} + \alpha_3\beta_3 x v^{\alpha_3} + \delta_3 v(x+y) - \delta_4 v - vx^2 - 2vxy - vy^2)(\alpha_2\beta_3 x v^{\alpha_3} - \alpha_2\beta_4 x v^{\alpha_4} + (\alpha_2-1)\delta_3 v(x+y) + \delta_4(v-\alpha_2 v) - \alpha_2 vx^2 - 2\alpha_2 vxy - \alpha_2 vy^2 - \alpha_3\beta_3 x v^{\alpha_3} + \alpha_4\beta_4 x v^{\alpha_4} + vx^2 + 2vxy + vy^2) + (\alpha_2\beta_2 x v^{\alpha_2-1} - \alpha_4\beta_4 y v^{\alpha_4-1})((\alpha_2-1)\beta_2 v^{\alpha_2}(\delta_4 - (x+y)(\delta_3 - x - y)) + (\alpha_3 - 1)\beta_3 v^{\alpha_3}(y(y-\delta_3) + \delta_4 - x^2) + (\alpha_4-1)\beta_4 y v^{\alpha_4}(\delta_3 - 2(x+y)))$,
- $D''(q) = (\beta_2 x v^{\alpha_2-1} - \beta_4 y v^{\alpha_4-1})(\alpha_2\beta_2 x v^{\alpha_2} + \alpha_3\beta_3 x v^{\alpha_3} + \delta_3 v(x+y) - \delta_4 v - vx^2 - 2vxy - vy^2) - (\alpha_2\beta_2 x v^{\alpha_2-1} - \alpha_4\beta_4 y v^{\alpha_4-1})(\beta_2 x v^{\alpha_2} + \beta_3 x v^{\alpha_3} + \delta_3 v(x+y) - \delta_4 v - vx^2 - 2vxy - vy^2)$,

and the singular control is given by: $u_s = -D'(q)/D(q)$.

*5.2.3. Stratification of the terminal manifold: $x = d$*
*Singular locus.* $\mathcal{S} : n \cdot [G,F](q) = 0$ and $x = d$ with $n = (1,0,0)$. It is given by:

$$\begin{aligned}\mathcal{S}:\ &\alpha_2\beta_2 d v^{\alpha_2-1} + \alpha_3\beta_3 d v^{\alpha_3-1} + d\delta_3 - \delta_4 \\ &\qquad - d^2 + y(\delta_3 - 2d) - y^2 = 0.\end{aligned} \tag{35}$$

Denoting by $\Delta$ the discriminant of the polynomial function $y \mapsto n \cdot [G,F](d,y,v)$, a singularity can occur for $\Delta = 0$.

One has

**Lemma 13.** *Assume $\alpha_i, \beta_i, \delta_i > 0$, i=1,2 and $d, v > 0$. Then we have $\Delta = (\delta_1 - \delta_2)^2 + 4d\,(\alpha_2\beta_2 v^{\alpha_2-1} + \alpha_3\beta_3 v^{\alpha_3-1}) > 0$ so that there is no ramification and $\mathcal{S}$ contains at most two real positive branches.*

**Definition 5.** *A semi-bridge occurs at a point $q \in \mathcal{S}$ if $n \cdot [[G,F],G](q) = 0$.*

Computing, a semi-bridge occurs if $v^{\alpha_3-\alpha_2} = -\frac{(\alpha_2-1)\alpha_2\beta_2}{(\alpha_3-1)\alpha_3\beta_3}$.

*Exceptional locus.* It is given by $\mathcal{E} : n \cdot F(q) = 0$ and $x = d$. Computing, one gets:

$$\begin{aligned}\mathcal{E}:\ &-\beta_2 d v^{\alpha_2} - \beta_3 d v^{\alpha_3} + d^2 v - d\delta_3 v \\ &\qquad + y\,(2dv - \delta_3 v) + \delta_4 v + vy^2 = 0.\end{aligned} \tag{36}$$

The discriminant of the polynomial $n \cdot X(q)$ in $y$ is $\Delta = v(4d(\beta_2 v^{\alpha_2} + \beta_3 v^{\alpha_3}) + v(\delta_1 - \delta_2)^2) > 0$ and $\mathcal{E}$ contains at most two real positive branches.

Fig.17 gives a picture of stratification of $x = d$ for the McKeithan system with a point where $\mathcal{S}$ is folded.

*Outline of the normalization.* We choose the coordinates $q = (x,y,z)$, the point $q_0$ is $(0,0,0)$ so that the system $\dot{q} = F(q) + u\,G(q)$, $|u| \leq 1$ is such that $N : \{x = 0\}$, $G = \frac{\partial}{\partial z}$ and we have the following:

- the set $\mathcal{S} \cap N : n \cdot [G,F](q) = 0,\ x = 0$ is $y = z^2$,
- the point $q_0$ satisfies $n \cdot [[G,F],G](q_0) = 0$ and $n \cdot [[G,F],F](q_0) \neq 0$,
- the trajectory associated to $u = 0$ defined on $[t_f, 0]$ with $\gamma(0) = 0$ is $\gamma : t \mapsto (t,0,0)$.

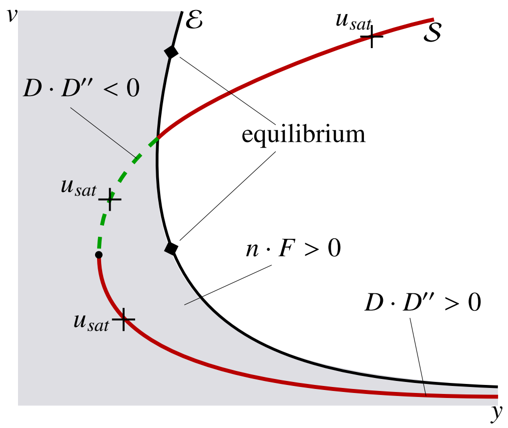


Figure 17: Stratification of the surface $x = d$ for the McKeithan reaction. Dotted line: elliptic, red line: hyperbolic.

We write

$$\begin{aligned}\dot{x} &= 1 + a\,y + b\,yz + c\,z^3 + \varepsilon_1(x,y),\\ \dot{y} &= d\,z + \varepsilon_2(x,y,z),\\ \dot{z} &= u + \varepsilon_3(x,y,z), \qquad |u| \le 1\end{aligned} \tag{37}$$

where $\varepsilon_1(x,y,z) = \sum_{i\ge1} a_i(x)\,y^i$, $a_1(0) = 0$, $\varepsilon_2(x,y,z) = \sum_{i+j\ge1} b_{ij}(x)\,y^i z^j$, $b_{01}(0) = 0$, $\varepsilon_3(x,y,z) = \sum_{i+j\ge1} c_{ij}(x)\,y^i z^j$.

Assuming $\varepsilon_i = 0$, we have

$$\begin{aligned}n \cdot [G,F](q) &= -b\,y - 3c\,z^2,\\ n \cdot [[G,F],G](q_0) &= 0,\\ n \cdot [[G,F],F](q_0) &= a\,d.\end{aligned}$$

Moreover, along $\mathcal{S}$ we have $D(q) \cdot D''(q) = -6cd^2\,z$ and the singular control is given by

$$u_s(q) = \frac{a\,d}{6\,c}\,\frac{1}{z}.$$

Since the system $(F, G, N)$ is normalized, we have

$$b = -3\,c \neq 0,\ \ d \neq 0,\ \ a \neq 0.$$

Also in a neighborhood of $q_0$ and along $\mathcal{S}$, we can choose $c > 0$ so that the set $\mathcal{S}$ splits into hyperbolic for $z < 0$ and elliptic for $z > 0$.

Fig.18 gives the stratification of $N$ near the $q_0$ for the system (37) where $a = 1$, $c = 1$, $b = -3$, $d = 1$ and $|u| \le 5$ and where the terms $\varepsilon_i$, $i = 1, 2, 3$ are zeros.

## 6. Conclusion

In this article, we have presented the mathematical tools from geometric optimal control to maximize the production of chemical networks using temperature control with applications to two test-bed cases concerning two reactions schemes.

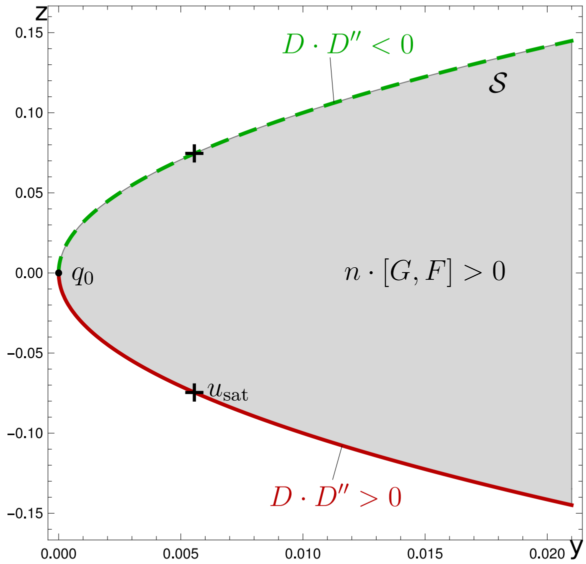


Figure 18: Stratification of $N$ for the system (37). Green dotted line: elliptic, red line: hyperbolic, crosses: saturating values of the singular control.

A brief recap of the dynamics is presented at constant temperature using the Feinberg-Horn-Jackson graph and is shown to be simple using the zero deficiency assumption.

The optimal control problem is analyzed in the frame of singularity theory and a first crucial step is to make the calculation of the closed loop optimal control for a time minimal control problem for which the terminal manifold is of codimension one and for a single input system. A classification of the local optimal syntheses is presented based on generic assumptions on Lie brackets relations. It is obtained from on explicit computations using adapted coordinates to simplify the calculations which amount to compute semi-normal form.

This approach is shown to be relevant to applications, since the classification can be used for different chemical networks. It is tested on two important schemes for applications: a sequence of two irreversible reactions and the McKeithan scheme. The classification presented in this article allows to completely solve the first case and has to be completed to make a complete analysis of the McKeithan scheme. Such completion is a good exercise for the reader to check if the tutorial objective of this article is fulfilled.

Additionally, for the first case a complete global solution of the problem is obtained based on a description of the (global) switching policy. For the McKeithan network, there is a serious difficulty to fulfill this scope which is revealed by the complexity of the singular flow, which contains in particular many singularities. They have to be analyzed in relation with the bridge phenomenon and the existence of equilibria. This is an important and challenging mathematical problem.

Note also that the graph structure of the network is not exploited directly in the optimal problem. It can be an important issue to handle the computational analysis of the Lie algebra structure associated to the system, which is crucial to understand the optimal control problem. This paves the road for further studies to deal in particular with nonzero deficiency network.

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