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1

Towards Geometric Time Minimal Control without Legendre Condition and with Multiple Singular Extremals for Chemical Networks

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Summary. This article deals with the problem of maximizing the production of a species for a chemical network by controlling the temperature. Under the so–called mass kinetics assumption the system can be modeled as a single–input control system using the Feinberg–Horn–Jackson graph associated to the reactions network. Thanks to Pontryagin's Maximum Principle, the candidates as minimizers can be found among extremal curves, solutions of a (non smooth) Hamiltonian dynamics and the problem can be stated as a time minimal control problem with a terminal target of codimension one. Using geometric control and singularity theory the time minimal syntheses (closed loop optimal control) can be classified near the terminal manifold under generic conditions. In this article, we focus to the case where the generalized Legendre-Clebsch condition is not satisfied, which paves the road to complicated syntheses with several singular arcs. In particular, it is related to the situation for a weakly reversible network like the McKeithan scheme of two reactions:

$$\begin{tikzcd} T+M \arrow[r, bend left] & A \arrow[l, bend left] \arrow[r] & B \arrow[ll, bend left] \end{tikzcd} .$$

Keywords:

Mass action chemical systems · Pontryagin Maximum Principle · Geometric optimal control · Time minimal synthesis · McKeithan type chemical scheme

Mathematics Subject Classification:

49K15 · 58K45 · 92B05

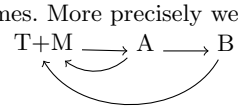
1 Introduction

The optimization of the production is an important problem in chemical and biological engineering and the control can be either the temperature (batch or closed

reactor) or by feeding the reactor (semi-batch or open case). In this article we shall concentrate on the first case. Moreover we assume that the dynamics is modeled using the mass action kinetics assumptions and hence given at constant temperature T by a polynomial system based only on the Feinberg–Horn–Jackson graph associated to the chemical network. Also in the 70's those researchers obtained (under the so–called zero deficiency assumption) in a series of seminal articles [17, 18] a complete description of the dynamics, at constant temperature. If this dynamics is well understood, in the optimal problem the temperature is not constant and the analysis becomes very intricate. Thanks to the Pontryagin Maximum Principle [24] candidates as minimizers can be found among extremals solutions of a (*non smooth*) Hamiltonian dynamics and optimal solutions are concatenation of bang arcs, with minimum and maximum temperature, and the so–called singular arcs, defined as a solution of a *smooth* Hamiltonian *constrained* dynamics [5]. Moreover maximizing the production of one species during the batch can be restated as producing a fixed amount of this species while minimizing the batch duration. In this frame, the problem is a time minimal control problem, with a terminal target manifold of *codimension one*.

For applications, the time optimal control has to be computed as a closed loop feedback and this leads to the problem of computing the time minimal *synthesis*, for a single–input control system. At the end of the 80's, geometric optimal control has produced an important literature to compute the time minimal syntheses for the *fixed end point case*, where the initial point is localized near the terminal point. This was done using the *Lie algebraic structure* of the control system, mainly for single–input (smooth) system, where the control appears linearly, some seminal references are [28, 26, 12] either in general context or in view of application formed by a sequence of two irreversible reactions: $A \to B \to C$ and in relation with an industrial project [8].

Our aim is to extend this work to more complicated reaction schemes and to deal in particular with weakly reversible chemical schemes. More precisely we shall concentrate on a McKeithan type scheme of the form



assuming that the coefficient governing the dynamics are given by Arrhenius law. This scheme was already studied in the context of control theory using stabilization techniques with "*feeding*" types control [27] and ad hoc *observer design* [14]. In our case, this network is a test bed case for our very general approach.

The key point for this extension is the analysis of singular trajectories and their role in the synthesis. This is connected with an important question and the need to extend the standard synthesis related to the turnpike phenomenon [29] to deal with cases, where the strict Legendre–Clebsch condition is not satisfied, a situation encountered in a recent application in MRI [6].

The organization of this article is the following. In Section 2, we recall briefly the Feinberg–Horn–Jackson theory to model the dynamics of chemical networks of constant temperature and the properties of the dynamics under the zero deficiency assumption [17, 18], which can be applied to the McKeithan scheme. The stability properties are recalled and can be applied to control stabilization and observer design [27, 14]. In Section 3, we present the fundamental results of the time minimal control problem, which are relevant to our study: Pontryagin Maximum Principle [24], regular and singular extremals [5],[20]. The general turnpike theorem [29] is

recalled and extensions are presented in relation with the problem with terminal manifold of codimension one and when the strict Legendre–Clebsch condition is not satisfied. The concept of conjugate and focal points is introduced based on [7]. In Section 4, we analyze the time minimal control problem for a two reactions McKeithan scheme. To compute the time minimal syntheses, we present techniques and results from [8, 9], which have to be extended to analyze the problem. The computational complexity of the problem is discussed and symbolic computations are presented to cope with this complexity.

2 Mathematical model and stability properties of the McKeithan network

2.1 Mass action kinetics networks and dynamics using the Feinberg–Horn–Jackson graph ([17],[18])

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

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

where α_i, β_i are the *stoichiometric coefficients* and the vectors $y = (\alpha_1, \ldots, \alpha_m)^\intercal$ and $y' = (\beta_1, \ldots, \beta_m)^\intercal$ are 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 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:

$$\begin{aligned} &K(y \to y') = k(T)\, c^y, \\ &c^y = c_1^{\alpha_1} \ldots c_m^{\alpha_m} \end{aligned} \tag{1.1}$$

and

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

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 different rate formulae can be used to deal in particular with biomedical systems (see for instance [27]). The dynamics of the system, taking into account the whole network is:

$$\dot{c}(t) = f(c(t), T) = \sum_{y \to y'} K(y \to y')\,(y' - y). \tag{1.2}$$

2.2 More explicit representation of the dynamics

Definition 1. *The stoichiometric subspace is* $S \coloneqq \operatorname{span}\{y - y';\ y \to y' \in \mathcal{R}\}$ *and the sets* $(c(0) + S) \cap \mathbb{R}^m_{\geq 0}$ *are called the (strictly if* > 0*) positive stoichiometric compatibility classes.*

From [2] we have.

Lemma 1. *Let $c(t)$ be a solution of (1.2) with initial condition $c(0) \in \mathbb{R}^m_{\geq 0}$. Then $c(t)$ belongs for all $t \geq 0$ to the strictly positive compatibility class $(c(0)+S) \cap \mathbb{R}^m_{\geq 0}$.*

Definition 2. *Having labeled the set of vertices by $i = 1, \ldots, n$, with corresponding stoichiometric vector $(y_1, \ldots, y_n)$, the complex matrix is $Y \coloneqq (y_1, \ldots, y_n)$. The incidence connectivity matrix $A \coloneqq (a_{ij})$ contains the Arrhenius coefficients k_i of the reactions using the rule: $k_1 = a_{21}$ indicates a reaction with kinetics constant k_1 from the first node to the second, that is $y_1 \underset{k_1}{\rightarrow} y_2$.*

With the mass kinetics assumption, the dynamics can be expressed as

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

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

$$\tilde{A} = A - \operatorname{diag}\left(\sum_{i=1}^{n} a_{i1}, \ldots, \sum_{i=1}^{n} a_{in}\right) \tag{1.3}$$

and we denote

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

2.3 The McKeithan scheme ([23, 27])

It is given by the reaction scheme:

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

The matrix Y is given 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 $a_{21} = k_1,\ a_{1i} = k_{-1,i-2},\ i = 2, \ldots, m$ $(m = N+2)$, $a_{i,i-1} = k_{p,i-3},\ i = 3, \ldots, m$ and all others a_{ij} are zero.

The stoichiometric subspace is defined by:

$$\{c : T + C_0 + \ldots + C_N = M + C_0 + \ldots + C_N = 0\}$$

and we note: $\delta_1 = T + C_0 + \ldots + C_N$ and $\delta_2 = M + C_0 + \ldots + C_N$ the constants associated to first integrals of the dynamics.

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

$$\begin{tikzcd} \mathrm{T{+}M} \arrow[r, bend left, "k_1"] & \mathrm{A} \arrow[l, bend left, "k_3"] \arrow[r, "k_2"] & \mathrm{B} \arrow[ll, bend left, "k_4"] \end{tikzcd}$$

, and restricting to the stoichiometric class (δ_1 and δ_2 being fixed), one gets with: $x := [A], y := [B]$, $[\cdot]$ denoting the respective concentrations, that the dynamics is described by the equations

$$\begin{aligned} \dot{x} &= k_1(\delta_1 x - y)(\delta_2 - x - y) - (k_2 + k_3)x \\ \dot{y} &= k_2 x - k_4 y. \end{aligned} \tag{1.4}$$

Definition 3. *The deficiency of the network is: $\delta = n - l - s$, where n is the number of vertices, l is the number of connected components and s is the dimension of the stoichiometric subspace. The network is called strongly connected 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.*

Using [17], refined by [2, 27], one has the following result.

Theorem 1. *The graph associated to the McKeithan scheme is strongly connected and with deficiency zero. In each strictly positive compatibility class there exists in this domain an unique globally asymptotically stable equilibrium.*

2.4 Application to stabilization and observer design for the McKeithan scheme

This stability result has consequences to control and observation properties of the network, see [27, 15], that we recall briefly. The dynamics (1.4) can be converted into a control system of the form

$$\begin{aligned} \dot{c}(t) &= f(x(t)) + u(t) \\ y(t) &= h(c(t)), \end{aligned} \tag{1.5}$$

where $u(\cdot)$ is a feeding control and h is a polynomial observation function.

Asymptotic stability of equilibrium in each strictly positive compatibility class will allow to get stabilization result for a single equilibrium. Moreover it leads to design under a mild assumption (detectability) a simple observer. We refer to [27] and [14] for the detailed presentation of those results, the geometric construction being clear.

3 The optimal control problem and Pontryagin Maximum Principle

3.1 Statement and notation for the optimal control problem

The system is written as $\frac{\mathrm{d}c}{\mathrm{d}t} = f(c, T)$ (see (1.4)) and controlling the temperature leads to $T \in [T_m, T_M]$. In the sequel, we shall use the terminology *direct* for the corresponding control problem. In practice, thermodynamics has to be used to model

the heat exchanges, in relation with the heat produced by the reactions [31] or the heat exchange device used in the experiments, depending upon the technical achievements. To avoid this part of the study and without losing any mathematically generality, we shall use $\dot{v}$ as the control variable setting $\dot{v} = u$, where $v := k_i(T)$ for some reaction i, where $k_i(T) = A_i e^{-E_i/(RT)}$ (see (1.1)). This leads to deal with the so–called *indirect* control system:

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

where $q = (c, v) \in \mathbb{R}^n$ is the extended state variable, $F = f(c, v)\, \frac{\partial}{\partial q}, G = \frac{\partial}{\partial v}$, $u_- \leq u \leq u_+$, where $[u_-, u_+]$ can be normalized to $[-1, +1]$. Note that the bounds $v \in [v_m, v_M]$ will not be taken into account in our study. The map $v \mapsto \dot{v}$ is the standard *Goh transformation* in optimal control, see [5].

The optimal control problem of physical interest is the problem of maximizing the production of one species and using a proper variable labeling, the optimal problem is therefore of the *Mayer type*:

$$\dot{q} = F(q) + u\, G(q), \quad \max_{|u| \leq 1} q_1(t_f),$$

where t_f is the time duration of the batch and q_1 is the desired product.

Note it will be show (thanks to the Maximum Principle) that a "dual" formulation is

$$\min_{u(\cdot)} t_f, \quad c_1(t_f) = d,$$

where $d > 0$ is the desired amount of the species X_1 during the batch.

3.2 Maximum Principle [24]

3.2.1 Notations and concepts

Consider a general control system of the form

$$\dot{q} = X(q, u), \quad q \in \mathbb{R}^n,$$

where X is a real analytic (C^ω) and the control is $u : [0, t_f(u)] \mapsto [-1, 1]$. The set of admissible controls $\mathcal{U}$ is the set of bounded measurable mappings. If $q(0) = q_0$ (initial state), we denote by $q(\cdot, q_0, u)$ (in short $q(\cdot)$) the solution starting from q_0. Fixing t_f, the *accessibility set* in time t_f is the set $A(q_0, t_f) = \bigcup_{u(\cdot) \in \mathcal{U}} q(t_f, q_0, u)$. The *extremity mapping* (in time t_f) is the map: $E^{q_0, t_f} : u(\cdot) \mapsto q(t_f, q_0, u)$ defined on a domain of $\mathcal{U}$; the set $\mathcal{U}$ is endowed with the L^∞-norm topology.

3.2.2 Pontryagin Maximum Principle (PMP)

Statement in the time minimal case with $q(t_f) \in N :=$ smooth terminal manifold.
Notation: $H(q, p, u) = p \cdot X(q, u)$ denotes the *pseudo–Hamiltonian* (Hamiltonian lift of the vector field X), p is the adjoint vector in $\mathbb{R}^n \setminus \{0\}$ and $\cdot$ is the scalar product. We denote by $M(q, p) = \max_{|u| \leq 1} H(q, p, u)$.

Statement of the PMP: If (q^*, u^*) is an optimal control–trajectory pair on $[0, t_f^*]$ then there exists $p^* \in \mathbb{R}^n \setminus \{0\}$ such that a.e.:

$$\begin{aligned} &\dot{q}^*(t) = \tfrac{\partial H}{\partial p}(q^*(t), p^*(t), u^*(t)), \\ &\dot{p}^*(t) = -\tfrac{\partial H}{\partial q}(q^*(t), p^*(t), u^*(t)), \\ &H(q^*(t), p^*(t), u^*(t)) = M(q^*(t), p^*(t)). \end{aligned} \tag{1.6}$$

Moreover $M(q^*(t), p^*(t))$ is a positive constant and p^* satisfies the *transversality condition*

$$p^*(t_f) \perp T_{q^*(t_f)}N. \tag{1.7}$$

Statement in the Mayer case: As before, except that the transversality condition is replaced by

$$p^*(t_f) = \frac{\partial \varphi}{\partial q}(x^*(t_f)),$$

where φ is the Mayer cost function to minimize.

Definition 4. *An extremal (q, p, u) is a solution of (1.6) on $[0, t_f]$. It is called a BC–extremal is $q(0) = q_0$ and $p(t_f)$ satisfies the transversality condition. An extremal control is called regular if $|u(t)| \leq 1$ a.e. and singular if $\frac{\partial H}{\partial u} = 0$ everywhere. An extremal is said exceptional if $M = 0$. A regular extremal control is called "bang–bang" if $u(\cdot)$ is piecewise constant on $[0, t_f]$ (i.e. the number of switches is finite).*

3.2.3 Computations of singular extremals

First case. Consider the case $\dot{q} = X(q, u)$, where $H = p \cdot X(q, u)$ and the condition $\frac{\partial H}{\partial u} = 0$ is satisfied. Denote by $z(\cdot) = (q(\cdot), p(\cdot))$ the reference extremal. From the maximization condition, the *Legendre–Clebsch condition* $\frac{\partial^2 H}{\partial u^2} \leq 0$ has to be fulfilled. If this inequality is strict, one can use the implicit function theorem to compute the singular control as the dynamic feedback: $z \mapsto u_s(z)$ and plugging such u_s into $H(q, p, u)$ leads to define the *true* (or maximized) Hamiltonian.
Second case. Let $\dot{q} = F(q) + u\,G(q)$. One introduces the following notations. If X and Y are two real analytic vector fields, 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 extremal lift of X is $H_X(z) = p \cdot X(q),\ z = (q, p)$ and the *Poisson bracket* is defined by $\{H_X, H_Y\}(z) = p \cdot [X, Y](q)$.
Computation of singular extremals:

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.*

Recall the following.

Proposition 1 ([19]). *The generalized Legendre–Clebsch condition is a necessary optimality condition for the time minimal control problem with fixed extremities.*

To compute the singular extremal, we differentiate twice $t \mapsto H_G(z(t))$ and we get

$$\begin{aligned} &H_G(z) = \{H_G, H_F\}(z) = 0, \\ &\{\{H_G, H_F\}, H_F\}(z) + u\,\{\{H_G, H_F\}, H_G\}(z) = 0. \end{aligned} \tag{1.8}$$

Assume (in relation with the Legendre–Clebsch condition) $\{\{H_G, H_F\}, H_G\} \neq 0$. The corresponding extremal is called of *order 2* and the singular control u is computed as $u_s(z)$, using relation (1.8). Plugging such $u_s(z)$ into $H(q, p, u)$ leads to define the *true* singular Hamiltonian, denoted by $H_s(z)$. One has:

Proposition 2. *Singular extremals of order* 2 *are the solutions of :*

$$\frac{\mathrm{d}q}{\mathrm{d}t} = \frac{\partial H_s}{\partial p}(z), \ \frac{\mathrm{d}p}{\mathrm{d}t} = -\frac{\partial H_s}{\partial q}(z) \tag{1.9}$$

with the constraints

$$\{H_G, H_F\}(z) = H_G(z) = 0.$$

Moreover, in order to be admissible, the singular control is given by

$$u_s(z) = -\frac{\{\{H_G, H_F\}, H_F\}(z)}{\{\{H_G, H_F\}, H_G\}(z)} \tag{1.10}$$

and has to satisfy the admissibility constraint $|u_s(z)| \leq 1$.

Definition 5. *Let $z = (q, p)$ 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).*

3.2.4 The case of chemical networks

Recall that for our network $\dot{c} = f(c, v)$, $v = k_i$ and it is extended into $\dot{q} = F(q) + u\,G(q)$ with $F = f(c, v)\frac{\partial}{\partial c}$ and $G = \frac{\partial}{\partial v}$. Denote $\tilde{H} = p_c \cdot f(c, v)$ and $H = p \cdot (F + u\,G)$ the respective Hamiltonian lifts, with $p = (p_c, p_v)$. One has the following relation between the corresponding singular extremals.

Lemma 2. *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, p_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

$$\frac{\mathrm{d}}{\mathrm{d}t}\frac{\partial H}{\partial u} = \{H_G, H_F\} = -\frac{\partial \tilde{H}}{\partial v} \tag{1.11}$$

$$\frac{\partial}{\partial u}\frac{\mathrm{d}^2}{\mathrm{d}t^2}\frac{\partial H}{\partial u} = \{\{H_G, H_F\}, H_G\} = -\frac{\partial^2 \tilde{H}}{\partial v^2}. \tag{1.12}$$

In particular this gives the correspondence between both singular Hamiltonian and the respective Legendre–Clebsch and generalized Legendre–Clebsch conditions.

3.2.5 The case $n = 3$

We have $q = (x, y, v)$ and introduce the following determinants:

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

Using $p \cdot G = p \cdot [G, F] = p \cdot ([[G, F], F] + u\,[[G, F], G]) = 0$ and eliminating p leads to the following.

Proposition 3. *If $n = 3$, the singular control is given by the feedback $u_s(q) = -D'(q)/D(q)$ and singular trajectories are defined by the vector field $X_s(q) = F(q) - \frac{D'(q)}{D(q)}\,G(q)$. Singular trajectories are hyperbolic if $DD'' > 0$, elliptic if $DD'' < 0$ and exceptional if $D'' = 0$.*

Optimality status: the case $n = 3$. We use [7] to describe the optimality status of singular trajectories. The system is $\dot{q} = F + u\,G$ and we relax the bound $|u| \leq 1$, assuming $u \in \mathbb{R}$ so that singular arcs are admissible. We assume the following:

(H_0) F, G are linearly independent,
(H_1) $G, [G, F]$ are linearly independent.

One picks a smooth singular arc $z(\cdot) = (q(\cdot), p(\cdot))$ defined on $[0, t_f]$ so that p is unique up to a non zero multiplicative scalar and $q(\cdot)$ is a one-to-one immersion. We have:

Proposition 4. *There exists a C^0–neighborhood U of the reference singular arc $t \mapsto q(t),\ t \in [0, t_f]$ so that $q(\cdot)$ is time minimal (resp. maximal) if $q(\cdot)$ is hyperbolic (resp. elliptic) up to the first conjugate time t_{1c} with respect to all trajectories with the same extremities contained in $\mathcal{U}$. In the exceptional case, the reference singular arc is time minimal (and time maximal).*

Algorithm to compute the first conjugate point in the hyperbolic–elliptic case. Let $V(t),\ t \in [0, t_f]$ be the solution of the *(variational) Jacobi equation*:

$$\dot{\delta q}(t) = \frac{\partial X}{\partial q}(z(t))\,\delta q(t)$$

with initial condition $V(0) = G(q(0))$, where $t \to q(t)$ is the reference singular arc. The first conjugate point t_{1c} is the first $t > 0$ such that $V(t)$ is collinear to $G(q(t))$.

See [5, p. 123] for a proof and the geometric interpretation.

3.3 Small time classification of regular extremals

In this section, we recall the seminal results coming from singularity theory due to [16, 20] to analyze the small time extremal curves near the switching surface.

Definition 6. *We denote by σ_+ (resp. σ_-) a bang arc with constant control $u = 1$ (resp. $u = -1$) and σ_s an admissible singular arc. We denote by $\sigma_1\sigma_2$ an arc σ_1 followed by σ_2. The surface $\Sigma : H_G(z) = 0$ is called the switching surface and let $\Sigma' \subset \Sigma$ given by $H_G(z) = \{H_G, H_F\}(z) = 0$. Let $z(\cdot) = (q(\cdot), p(\cdot))$ be a reference curve on $[0, t_f]$. We note $t \mapsto \Phi(t) := H_G(z(t))$ the switching function, which codes the switching times.*

Deriving twice with respect to time the switching function, one gets

$$\dot{\Phi}(t) = \{H_G, H_F\}(z(t)), \tag{1.13}$$

$$\ddot{\Phi}(t) = \{\{H_G, H_F\}, H_F\}(z(t)) + u(t)\,\{\{H_G, H_F\}, H_G\}(z(t)). \tag{1.14}$$

From this, we derive.

Lemma 3. *Assume that t is an ordinary switching time, that is $\Phi(t) = 0$ and $\dot{\Phi}(t) \neq 0$. Then near $z(t)$ every extremal projects onto $\sigma_+\sigma_-$ if $\dot{\Phi}(t) < 0$ and $\sigma_-\sigma_+$ if $\dot{\Phi}(t) > 0$.*

The situation is more complex for higher contact with Σ.

Definition 7. *The fold case is characterized by $\Phi(t) = \dot{\Phi}(t) = 0$ and $\ddot{\Phi}(t) \neq 0$ (replacing u by ± 1 in (1.14)). Hence $z(t) \in \Sigma'$. Assume that locally Σ' is a regular surface of codimension two. We have three cases:*

- *Parabolic case: $\ddot{\Phi}_+(t)\ddot{\Phi}_-(t) > 0$.*
- *Hyperbolic case: $\ddot{\Phi}_+(t) > 0$ and $\ddot{\Phi}_-(t) < 0$.*
- *Elliptic case: $\ddot{\Phi}_+(t) < 0$ and $\ddot{\Phi}_-(t) > 0$.*

Denote by $u_s(\cdot)$ the singular control defined by (1.14) as $\ddot{\Phi}(t) = 0$. In the hyperbolic case, through $z(t)$, assuming $\{\{H_G, H_F\}, H_G\}(z(t)) \neq 0$, there exists a singular arc, which is strictly admissible that is $|u_s(t)| < 1$. This arc is hyperbolic if $\{\{H_G, H_F\}, H_G\}(z(t)) > 0$ (strict Legendre–Clebsch condition) and elliptic if this quantity is < 0. In the parabolic case, it can be absent or not admissible that is $|u_s(t)| > 1$.

One has from [20],

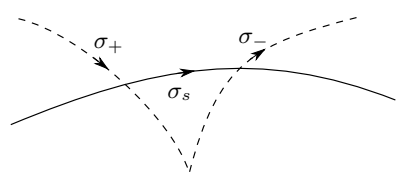


Fig. 1.1. Fold case in the elliptic 2D–situation and the antiturnpike phenomenon.

3.4 Global case

It is based on [7] and presented here for $n = 3$. It uses proposition 4. Under our assumptions $(H_0) - (H_1)$, and if moreover the singular control is *strictly admissible* on $[0, t_f]$, that is $|u_s(t)| < 1$, the reference singular arc can be immersed in a C^0–domain *up to the first conjugate time* t_{1c} and where the time minimal policy is of the form $\sigma_\pm\sigma_s\sigma_\pm$, see Fig. 1.2 for the interpretation of the first conjugate time t_{1c} for the problem in the q–space with $q = (c, v)$, $\dot{v} = u$.

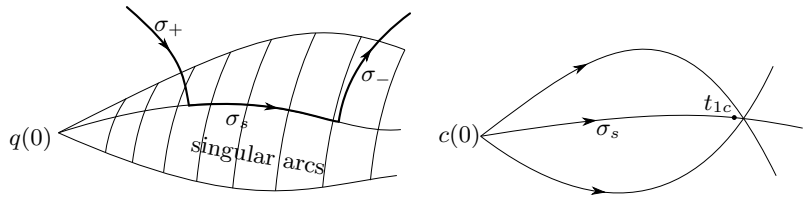


Fig. 1.2. *(left)* Time minimal policy in the q–space. *(right)* Conjugate point in the c–space.

3.5 The curse of the non strict Legendre–Clebsch condition

More complicated and challenging situation is to analyze situations, where the strict Legendre–Clebsch condition is not satisfied that is $\{\{H_G, H_F\}, H_G\}(z(t))$ vanishes at some times. Due to the complexity and in relation with our application, we shall assume that $n = 3$.

In this case, one has $D = 0$ since $\{\{H_G, H_F\}, H_G\} = p \cdot [[G, F], G]$ and recall that $D = \det(G, [G, F], [[G, F], G])$. The singular flow is defined by the vector field $X_s(q) = F(q) - \frac{D'(q)}{D(q)} G(q)$. Using a time reparameterization, it is related to the one–dimensional foliation $\mathcal{F}_s : D(q)F(q) - D'(q)G(q)$. Complexity of the analysis is due to *non isolated singularities* contained in the set $D'(q) = D(q) = 0$.

In relation with our optimal problem with terminal manifold N of codimension one given by $x = d$, our singularity resolution will be concerned by analyzing arcs initiating from the set $\mathcal{S} : n \cdot [G, F](q) = 0$, where $n = (1, 0, 0)$ is the normal vector to N. Singularities can be roughly classified into two types: local in relation with singularities of $\mathcal{S}$ and propagated along the singular flow, and Lagrangian singularities in relation with the concept of conjugate–focal points. This will be developed in the next section.

4 Geometric techniques to analyze the 2d–McKeithan Network

4.1 Time minimal syntheses near the terminal manifold

4.1.1 Notations and definitions

The system is written $\dot{q} = F(q) + u\,G(q)$, $|u| \leq 1$, with $q = (c, v)$, $G = \frac{\partial}{\partial v}$. The terminal manifold N is given by $c_1 = d$. The problem is to determine *small time* synthesis near a given point $q_0 \in N$, which can be identified to 0. More precisely one wants to classify the syntheses under generic assumptions near the terminal manifold in relation with the Lie algebraic structure of $\{F, G\}$ at q_0. Our approach developed in our series of articles [10, 9, 8, 21] is to use the construction of *semi–normal form* for the action of the pseudo–group $\mathcal{G}$ of local diffeomorphisms and feedback transformation $u \to -u$ (so that σ_+ and σ_- can be exchanged). Additionally recall that the pseudo–group $\mathcal{G}_f$ formed by local diffeomorphims and feedback actions of the form $u = \alpha(q) + \beta(q)v$ leaves the singular flow invariant [4]. These groups act

on the jet space of F at zero, G being identified to $\frac{\partial}{\partial v}$ and the terminal manifold N to $c_1 = d$. Note that the problem is *flat* that is G is tangent to N. For the action of the pseudo–group G on the jet spaces of F we refer to [22] (we shall work in the C^k category, where $k \geq 1$ is not precised) and the semi–normal form is related to a semi–algebraic stratification on the jet spaces of (F, G, N). One has $N : c_1 = d$ and the initial state is such that $c_1(0) < d$. Denote in general $N^\perp = \{(q, p);\ p \cdot v = 0, \forall v \in T_q N\}$ and let n be the outward normal to N so that $n = (1, 0, \ldots, 0)$ and $N^\perp = (q, n(q))$. Let $z = (q, p)$ be a BC–extremal on $[t_f, 0]$, $t_f < 0$ and $z(0) \in N^\perp$ (this convention is used since we integrate *backwards* from the terminal manifold). The set of minimizing switching points can be stratified into stratum of *first kind* if the optimal curves are tangent and *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 trajectories loses its optimality, see [3, 13] for the introduction of those concepts in the frame of semi–analytic geometry.

We introduce the following triplet (F, G, N) in the C^ω–category, with $N = \{f(q) = 0\}$, where f is a (local) submersion. Fixing $q_0 \in \mathbb{R}^n$, we denote by $j_k F(q_0), j_k G(q_0), j_k f(q_0)$ the respective k–jets, that is the Taylor expansions at order k. We say that (F, G, f) has at q_0 a singularity of *codimension* i if $(j_k F(q_0), j_k G(q_0), j_k f(q_0)) \in \Sigma_i$, where Σ_i is a semi–algebraic submanifold of codimension i in the jets space.

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

4.1.2 Local syntheses: general tools and classification

We shall present the main steps to compute the time minimal syntheses, restricting our study to the 3-dimensional case, but it can be clearly extended to the n–space with the concept of codimension [21].

The system is written: $\dot{q} = F(q) + u\, G(q)$, $|u| \leq 1$ and let $q = (x, y, z)$ be the coordinates, G being identified to $\frac{\partial}{\partial z}$ and G being tangent to N, which can be identified to $x = 0$ and $n = (1, 0, 0)$ is the outward normal to N. Recall that (generic) singular trajectories are given by $\dot{q} = F(q) + u_s(q) G(q)$, $u_s(q) = -D'(q)/D(q)$ and they can be classified into: hyperbolic, elliptic, exceptional, see section 3.

The first step is to stratify the terminal manifold into:

- $\mathcal{S}$: *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 $q \in N$ so that $N^\perp \subset \Sigma$, where Σ is the switching surface.

Generic case. The first case is when $F(q_0)$ and $[G, F]\,(q_0)$ are independent and not tangent to N and the synthesis follows from Lemma 3. It is given by σ_+ if $n \cdot [G, F]\,(q_0) < 0$ and σ_- if $n \cdot [G, F](q_0) > 0$ since the final point is a *virtual* switching point.

Generic hyperbolic singular case and the concept of focal points. Now we present the basis of our analysis, the so–called hyperbolic situation. In this case, based on [9], a semi–algebraic normal form is constructed to obtain the corresponding local syntheses and it is extended (in the jet space) *along the reference singular arc*

in order to obtain the concept of *focal point* based on the notions of turnpike and conjugate points presented in Section 3.
Semi–normal form: one has $q_0 = 0$ and we make the following assumptions:

- The tangent space to N is $G(0)$, $[G, F](0)$.
- The set of points δ, 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 simple BC–singular extremal σ_s transverse to N. One can choose local coordinates so that G is identified to $\frac{\partial}{\partial z}$, δ to the axis (Oy) can be identified to $t \mapsto (t, 0, 0)$, whose image is the (Ox)–axis. Note that N is identified to $x = 0$.

The semi–normal form is constructed in a tubular neighborhood of the reference singular curve σ_s and the vector field F is developed in the jet space with respect to (y, z) since $\sigma_s : t \mapsto (t, 0, 0)$ is the x–coordinate. One has the following semi-normal form

$$\begin{aligned}
\dot{x} &= 1 + a(x)z^2 + 2b(x)yz + c(x)y^2 + R_1 \\
\dot{y} &= d(x)y + e(0)z + R_2 \\
\dot{z} &= (u - u_{s|\sigma}(x)) + f(x)y + g(0)z + R_3,
\end{aligned}$$

where $a(x) \neq 0,\ e(0) \neq 0$ and R_1 (resp. $R_2,\ R_3$) are terms of order ≥ 3 (resp. ≥ 2) in (y, z) and u_s is the singular control.

Furthermore we make the following assumption:

- The reference arc is *hyperbolic* on $[t_f, 0]$ so that $a(x) < 0$.

According to [9] the time minimal synthesis near q_0 is of the form $\sigma_+\sigma_s\sigma_-$, see Fig.1.3 and is described by the unfolding

$$\begin{aligned}
\dot{x} &= 1 - a(0)\, z^2 \\
\dot{z} &= u - u_s(0) \\
\dot{y} &= 0
\end{aligned}$$

in a small neighborhood of $q_0 = 0$.

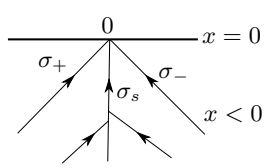


Fig. 1.3.

Local syntheses and the semi-bridge phenomenon.

We use [9] and the `Mathematica`'s program given in Appendix 6.1. One fixes a point $q_0 \in \mathcal{S}$ and we make the explicit computations of the switching and cut loci near q_0 using the jet expansion of F at q_0, G and N being normalized respectively to $\frac{\partial}{\partial v}$ and $x = 0$. The computations are in the semi-algebraic category, easily implementable using symbolic algorithms and the cut locus and switching loci are stratifiable.

Switching locus. We denote by K the set of ordinary switching points for BC-extremals, K_+ being a switching $\sigma_-\sigma_+$ and K_- being a switching $\sigma_+\sigma_-$, while W, W_+, W_- corresponds respectively to switching points of optimal extremals. More precisely, near N the stratification of W is $W = W_1 \cup W_2$ where W_1 is the first kind stratum composed by the hyperbolic singular arcs and $W_2 = W_s \cup W_+ \cup W_-$ is the second kind strata, where $W_\varepsilon,\ \varepsilon \in \{-1, 1\}$ is composed by the ordinary switching points of the policy $\sigma_{-\varepsilon}\sigma_\varepsilon$ and W_s is the first switching point of the Bang-Bang-Singular's policy.

From [1] we have two situations describe by Fig.1.4. The reflecting case corres-

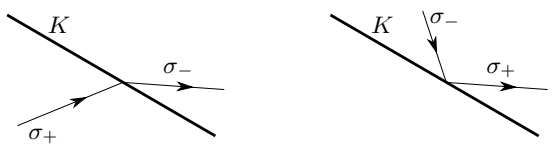


Fig. 1.4. *(left)* Crossing. *(right)* Reflecting.

ponds to a non optimal situation and has to be rejected to determine W.

Using the theory and computations of [9] only the stratification of W localized near q_0 can be computed.

Singular locus. Near q_0, one determines the singular locus Γ_s restricting to admissible singular trajectories, which are optimal. In other words, the test is : hyperbolicity and strict admissibility $|u_s| < 1$.

Cut locus. The cut locus C is the set of points where optimality is lost. One part of the cut locus is formed by the splitting locus L, where two minimizers intersects. It can be stratified into strata corresponding between intersections σ_+, σ_- intersections between $\sigma_+\sigma_-$ and σ_- ... Again such intersections are described in [9].

The local syntheses.

It is based on the classification of section 3.3.

Generic case. Since G is tangent to N, every final point is a virtual switching point. Denoting $\Phi(t)$ the switching function on $[t_f, 0]$, with $\Phi(0) = n \cdot G(q_0)$ one has: if $\dot{\Phi}(0) := n \cdot [G, F](q_0) < 0$ (resp. > 0) the terminating arc is σ_- (resp. σ_+).

Codimension one case. We have different cases corresponding to the fold case, since in the parabolic case one must distinguish between a parabolic point corresponding either to a non admissible hyperbolic or elliptic arc. The cases are represented on Fig.1.5-1.6.

The syntheses can be represented by foliations by 2d-planes. Note that the role of σ_+ and σ_- can be interchanged since the semi-normal forms are computed using the transformation $u \mapsto -u$.

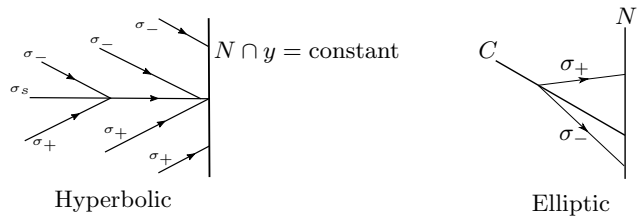


Fig. 1.5. Fold case.

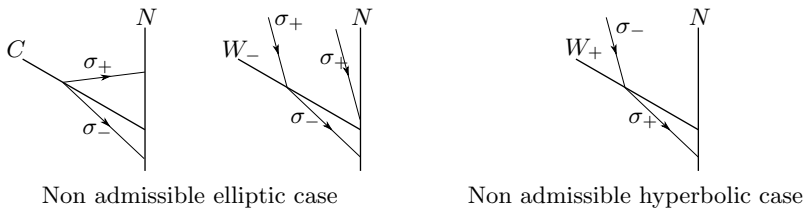


Fig. 1.6. Parabolic point with a non admissible singular arc.

The $\mathcal{C}^0$-unfoldings are:

- Hyperbolic and Parabolic:

$$\begin{aligned} \dot{x} &= 1 + a\,y^2 \\ \dot{y} &= u - u_s(0), \qquad |u_s(0)| < 1, \end{aligned}$$

  and $a < 0$ (hyperbolic) or $a > 0$ (elliptic).
- Parabolic:

$$\begin{aligned} \dot{x} &= 1 + a\,y^2 \\ \dot{y} &= u - u_s(0), \qquad |u_s(0)| > 1, \end{aligned}$$

  and $a \neq 0$.

Focal points.

The synthesis in the hyperbolic case can be extended to a tubular neighborhood of σ_s for $t \in [t_f, 0]$ introducing the concept of focal point as follows. By assumptions, $W := \delta'(0)$ belongs to $\text{span}\{G(0), [G,F](0)\}$. Let λ_1, λ_2 be two scalars such that $W = \lambda_1 G(0) + \lambda_2 [F,G](0)$ and by assumption $\lambda_1 \neq 0$. Denoting by $X_s(q) := F(q) - \frac{D'(q)}{D(q)} G(q)$, we introduce the variational equation

$$\dot{\delta q}(t) = \frac{\partial X_s}{\partial q}(\sigma_s(t))\,\delta q(t)$$

and let $W(\cdot)$ be a solution on $[t_f, 0]$ such that $W(0) = W$.

Definition 8. *Let t_{1f} be the first time in $[t_f, 0]$ such that:* $\det(W(t), G(\sigma_s(t)), F(\sigma_s(t))) = 0$. *Then t_{1f} is called the first focal point along σ_s.*

As for the fixed end point problem we have the following:

Proposition 5. *Provided $t \in]t_{1f}, 0]$, then in a tubular neighborhood of σ_s the set $S = \{\exp(tX_s(\sigma))\}$ is a smooth surface and the synthesis is given by Fig.1.3.*

Algorithm: Besides the definition, which leads to compute focal point using a singular value decomposition, an equivalent computation is to determine $t = t_{1f}$ such that $W(t)$ becomes collinear to $G(\sigma_s(t))$.

Two codimension-two cases.

The situation is more intricate. It is analyzed using the semi-normal form constructed in [9]. A model is

$$\begin{aligned} \dot{x} &= 1 + a\,z^2 + \alpha_1\,xy^2 + \alpha_2\,yz^2 + \alpha_3\,xz^2 \\ \dot{y} &= b\,z \\ \dot{z} &= c\,z - u_s(0) - u_{sx}\,x - u_{sy}\,y, \end{aligned} \tag{1.15}$$

where u_s is the singular control, $u_s(0) \in \{1, 3\}$, $u_{sx} = \frac{\partial u_s}{\partial x}(0)$, $u_{sy} = \frac{\partial u_s}{\partial y}(0) > 0$ and $a, b, c \neq 0$. The switching function $\Phi(t) := p_3(t)$ is developed at order 3 and factorized as $tP(t)$, where P is polynomial of order two with two roots t_1, t_2, which determine the switching points.

If $a > 0$, we are in the elliptic situation and if $a < 0$ in the hyperbolic situation and the reference singular arc is identified to $\sigma_s : t \mapsto (t, 0, 0)$ being not admissible. One has $|u_s(0)| > 1$ and we can assume $u_s(0) > 1$.

Figures presented in this section are obtained with the `Mathematica`'s program of Appendix 6.1, we use the following values: $\alpha_1 = \alpha_2 = \alpha_3 = u_{sy} = c = b = 1$.

The case $a > 0$ and $u_s(0) = 3$. We have the following three situations

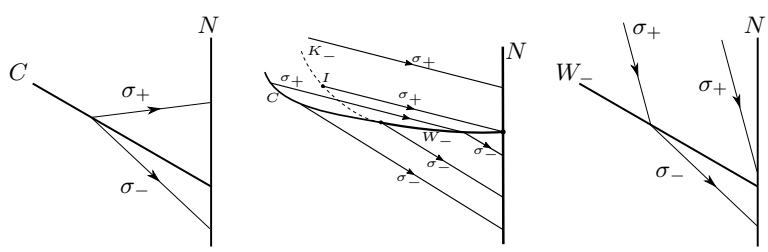
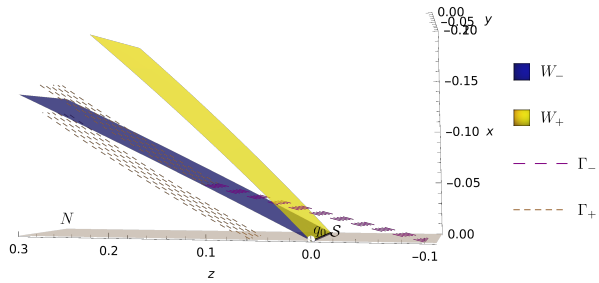


Fig. 1.7. Bifurcation of the cut ($a > 0$, $u_s(0) = 3$). The cut locus C splits into $C_1 \cup C_{12}$ where $C_1 : \sigma_- \cap \sigma_+$ and $C_{12} : \sigma_+\sigma_- \cap \sigma_-$.

Note that the cut appears when the trajectories reflect on the switching surface, see Fig.1.8.



$y < 0$

Fig. 1.8. A situation in the elliptic parabolic case. The trajectories of Γ_- reflect on W_- leading to a cut locus between W_- and W_+.

The case $a < 0$ and $u_s(0) = 1$. There are two generic cases described by Fig.1.9-1.10. The two cases are discriminated by the existence or not of the singular arc in the transition. In the second case, the switching locus Σ has two strata : $\Sigma = W_+ \cup W_s$, where W_+ corresponds to optimal policies $\sigma_-\sigma_+$ and W_s to policies $\sigma_-\sigma_+\sigma_s$, Σ is not C^1. The stratum $W_s \cup \Gamma_s$ is C^1 but not C^2.

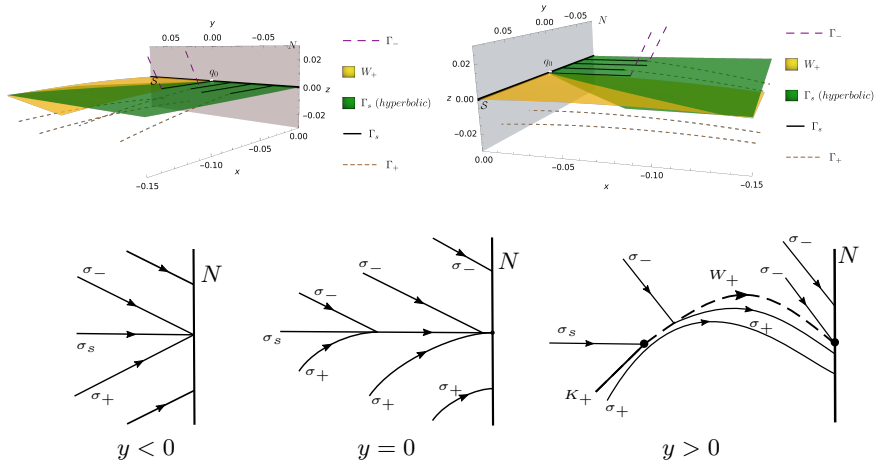


Fig. 1.9. Saturating case 1: $-1 = a < 0$, $1 = u_{sx} > 0$. Top figures are obtained using the `Mathematica`'s program given in the Appendix 6.1 and these situations are sketched in the bottom figures.

4.1.3 Beyond the strict generalized Legendre–Clebsch condition

In our previous work in the 90's we restricted our study to the case, where the strict generalized Legendre–Clebsch condition is satisfied, see [9]. Now our program is to extend this analysis when this condition is not satisfied.

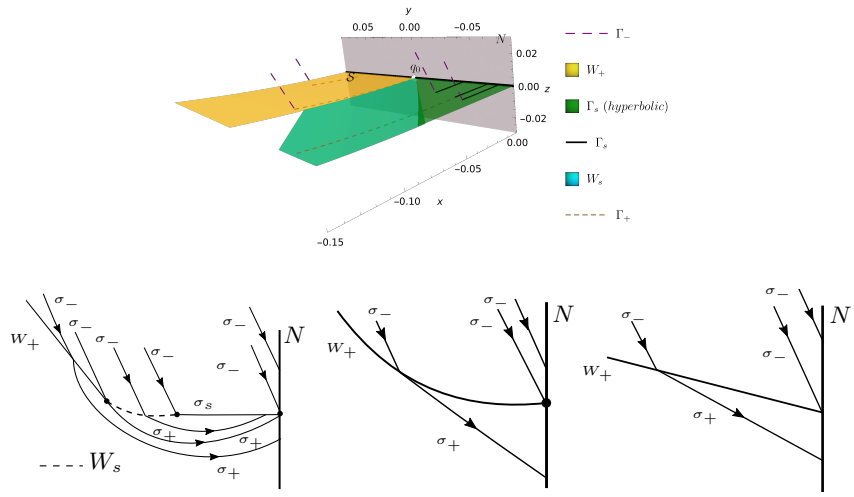


Fig. 1.10. Saturating case 2: $-1 = a < 0$, $1 = u_{sx} < 0$. Top figure is obtained using the `Mathematica`'s program given in the Appendix 6.1 and the corresponding situations are sketched in the bottom figures.

The semi–bridge phenomenon as transition between two saturations

A bridge in optimal control was introduced in [6] as a policy of the form Bang-Singular-Bang-Singular, where the second bang is related as a saturation due to the violation of the strict Legendre-Clebsch condition. In our context a semi–bridge is interpreted as a path to a bridge due to saturation between optimal singular arcs.

A tutorial model for the semi–bridge. Consider the case

$$\begin{aligned} \dot{x} &= 1 + a\,y - 3c\,yz + c\,z^3 \\ \dot{y} &= z \\ \dot{z} &= u, \qquad |u| \leq 1, \end{aligned} \tag{1.16}$$

where $a, c \neq 0$ are parameters.

Lie brackets computations. We have

$$\begin{array}{ll} F = (1 + ay - 3cyz + cz^3)\frac{\partial}{\partial x} + z\frac{\partial}{\partial y}, & G = \frac{\partial}{\partial z}, \\ [G, F] = 3c(y - z^2)\frac{\partial}{\partial x} - \frac{\partial}{\partial y}, & [[G, F], G] = -6cz\frac{\partial}{\partial x}, \\ [[G, F], F] = a\frac{\partial}{\partial x}, & D(q) = \det(G, [G, F], [[G, F], G]) = -6cz, \\ D'(q) = \det(G, [G, F], [[G, F], F]) = a, & D''(q) = \det(G, [G, F], F) = ay - 2cz^3 + 1. \end{array}$$

Stratification of N.
We have the following properties

- $N : x = 0$, $G = \frac{\partial}{\partial z}$
- $\mathcal{S} : n \cdot [G, F] = 0 \cap \{x = 0\}$ is the parabola: $y = z^2$.
- $n \cdot [[G, F], G](0) = 0$, $n \cdot [[G, F], F](0) \neq 0$.

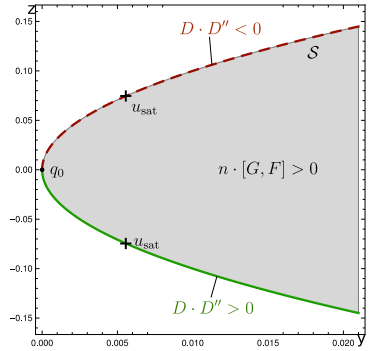


Fig. 1.11. Stratification of N for the system (1.16) ($a = c = 1$). Green dotted line: elliptic, red line: hyperbolic, crosses: saturating values of the singular control.

Observe that $\mathcal{E} : n \cdot F(q) = 0$ is the defined by $y(a - 3cz) + cz^3 + 1 = 0$.

One will localize our study in a neighborhood V of 0 such that: $\mathcal{E} \cap V = \emptyset$. We represent such a situation on Fig.1.11 One has $u_s = a/(6cz)$ and the points u_{sat} are given by $|u_s| = 1$.

We have two saturating points, one in the hyperbolic domain and one in the elliptic domain. Near the fold, the two saturation phenomenons are glued together using the curvature of $\mathcal{S}$, the normal to N being given by $n = (1, 0, 0)$, while q_0 follows $\mathcal{S}$. Note that since the control is blowing up at the fold, we encounter the case $a > 0, u_s(0) = 3$ (see Fig.1.7) and the bifurcation phenomenon of C, which splits into the case σ_+, σ_- and the case $\sigma_+\sigma_-$ and σ_- intersecting minimizers. The two strata will be denoted C_{12} and C_1. The model detects the two strata.

The stratification of the terminal manifold near the semi–bridge and the local time minimal synthesis are described in Fig.1.12.

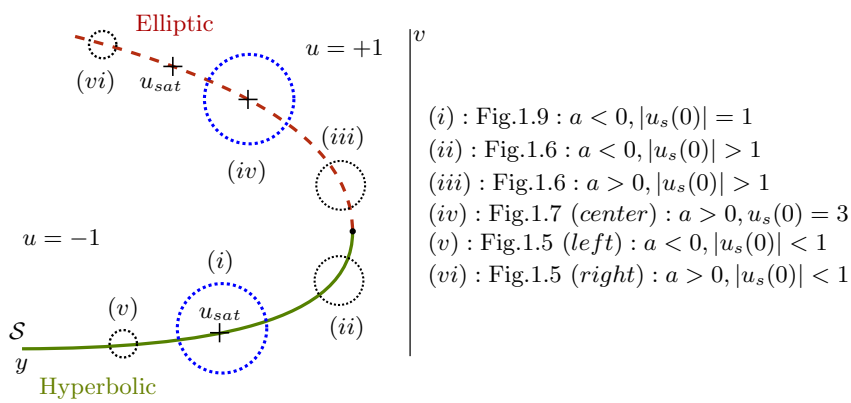


Fig. 1.12. Stratification of the target $x = 0$ for a semi–bridge model and the associated local syntheses.

Local syntheses by symbolic computations.

We use the `Mathematica`'s program in Appendix 6.1 to derive the local syntheses for the semi–bridge model.

We compute the time minimal synthesis in a neighborhood U of $q_0 \in N$ where $N : x = 0$ is the target. Since the problem is flat, q_0 is either an ordinary switching point, a fold point, or a codimension two case.

Denote n the unit normal of N at q_0 such that n belongs to the half-space containing the set $\{X + uY,\ |u| \leq 1\}$, i.e. $n = (1, 0, 0)$.

Assume $X(q_0)$ and $[Y, X](q_0)$ are not tangent to N. Then q_0 is an ordinary point and the optimal control is given by $u(q_0) = -\text{sign}\ p \cdot [Y, X](q_0)$.

We take $q_0 = (0, s_0^2, s_0)$ and we look at the behavior of BC-extremals reaching N near q_0. The switching surface W, the splitting locus C and the trajectories $\sigma_\pm$ are computed via symbolic computations, expanding the jets of F and G up to some order.

- Near a parabolic point on an hyperbolic singular arc.
  BC-extremals σ_- switch while BC-extremals σ_+ don't. These computations are represented in Fig. 1.13 for $q_0 = (0, (-0.05)^2, -0.05)$.
- Near a parabolic point on an elliptic singular arc.
  BC-extremals $\sigma_\pm$ reflect on the switching surface $W_\pm$, hence a cut locus appears between the switching surfaces. We represent in Fig. 1.14 with $q_0 = (0, 0.04^2, 0.04)$, $0.04 > z_{sat} = a/(6c)$ this cut locus and the switching surface W_-, together with the elliptic singular surface Γ_s.
- Near a saturated point on an hyperbolic singular arc.
  We have $q_0 = (0, z_{sat}^2, -z_{sat})$ where $z_{sat} = \frac{a}{6c}$. The synthesis is represented in Fig.1.15 and it corresponds to the synthesis described earlier by Fig.1.9.

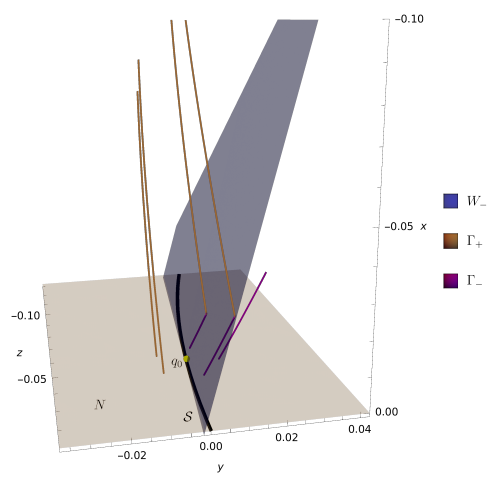


Fig. 1.13. Time minimal synthesis near an hyperbolic fold point for $q_0 = (0, (-0.05)^2, -0.05)$. Only the BC-extremals with optimal control -1 switch for the tutorial model (1.16) with $a = c = 1$. The tangent space of the switching surface at q_0 is represented.

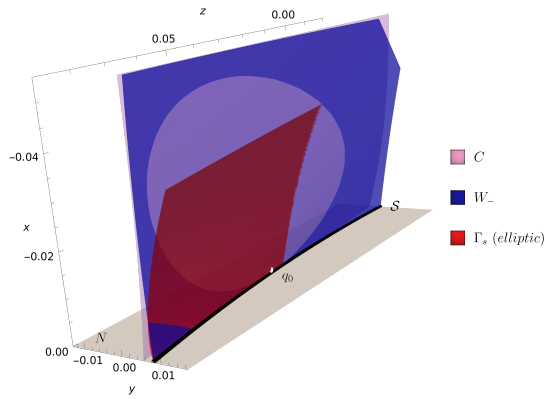


Fig. 1.14. Time minimal synthesis near an elliptic fold point for $q_0 = (0, 0.04^2, 0.04)$ for the tutorial model (1.16) with $a = 1$, $c = 5$.

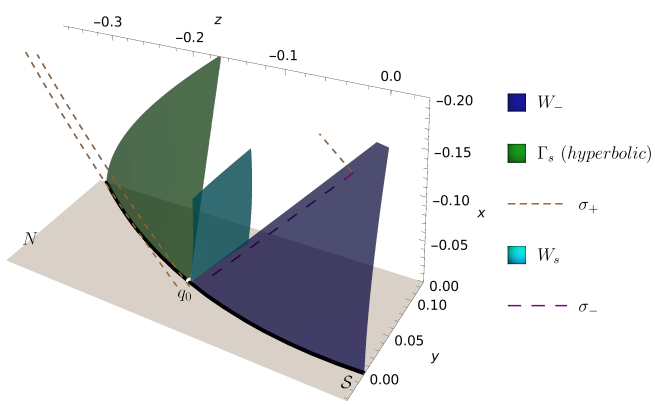


Fig. 1.15. Time minimal synthesis near a saturating hyperbolic fold point $q_0 = (0, z_{sat}^2, -z_{sat})$ for the tutorial model (1.16) with $a = c = 1$. Trajectories σ_- switch, while σ_+ don't. The surface W_s is the first switching point of the sequence $\sigma_+\sigma_-\sigma_s$.

These computations confirm the expected results and validate the symbolic program to investigate the McKeithan model.

Remark 1. We can investigate other singularities by the same method, for instance:

- Cusp singularity $y = z^3$.
- Singularity $y^2 = z^2$.
- Case $D = D' = 0$ is $q = \{0\}$.

Global analysis.

Take $u = \varepsilon \in \{-1, 1\}$. The dynamics (1.16) is integrable and we have

$$p_3(t) = \frac{1}{2} t \left(-2ct^2 + (a - 6c\varepsilon s_0)t - 6cs_0^2 + 6cw_0\right).$$

Denoting by $\Gamma_\varepsilon(q_0)$, $\varepsilon \in \{-1, 1\}$ the surface composed by the trajectories σ_ε passing through q_0, then $\Gamma_\varepsilon(0, w_0, s_0)$ is parameterized by

$$\begin{aligned} x =& t\left((a - 3cs_0) + cs_0^3 + 1\right) + \frac{1}{2}t^2\left(s_0(a - 3cs_0) + 3c\varepsilon(s_0^2 - w_0)\right) + o(t^3) \\ y =& w_0 + s_0 t + \frac{\varepsilon t^2}{2} + o(t^3) \\ z =& s_0 + \varepsilon t + o(t^3). \end{aligned}$$

Solving $p_3 = 0$ with respect to w_0, the switching surface K_ε for BC-extremals of controle $u = \varepsilon$ on N is parameterized by:

$$\begin{aligned} x =& \frac{1}{6}t^2\left(-\frac{a^2}{c} + 6a\varepsilon s_0 + 6as_0 - 18c\varepsilon s_0^2 - 9cs_0^2\right) + \frac{1}{6}t\left(6as_0^2 - 12cs_0^3 + 6\right), \\ y =& t\left((\varepsilon + 1)s_0 - \frac{a}{6c}\right) + \frac{1}{6}(3\varepsilon + 2)t^2 + s_0^2 \\ z =& s_0 + \varepsilon t + o(t^3). \end{aligned}$$

The switching condition of a trajectory on W_ε is given by the sign of

$$\det\left(\frac{\partial K_\varepsilon}{\partial t}_{|t=0}, \frac{\partial K_\varepsilon}{\partial t}_{|t=0}, \frac{\partial \Gamma_\varepsilon(0, s_0^2, s_0)}{\partial t}_{|t=0}\right),$$

and this determinant is equal to $\left(as_0^2 - 2cs_0^3 + 1\right)(6c\varepsilon s_0 - a)/(6c)$. In the case $a = c = 1$, we get that σ_+ (resp. σ_-) switches on W_+ (resp. W_-) for $z \in]z_{sat}, 1[$ (resp. $z \in]-z_{sat}, 1[$) as illustrated in Fig.1.16 (resp. Fig.1.17).

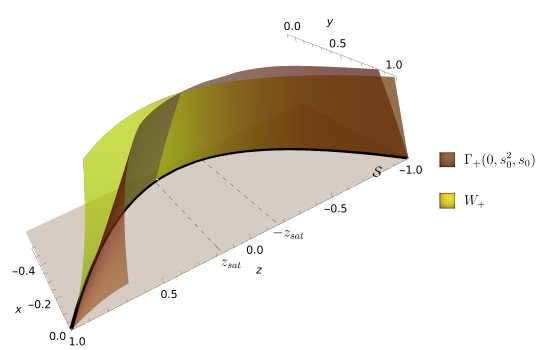


Fig. 1.16. The trajectories σ_+ starting from $q_0 = (0, w_0, s_0)$ such that $w_0 < s_0^2$ switch on W_+ for $z \in]z_{sat}, 1[$ $(a = c = 1)$.

We deduce the time minimal synthesis from Fig.1.18-1.19 for all point q_0 along $\mathcal{S}$. More precisely, if $z < -z_{sat}$ the optimal policy is Bang-Singular-Bang; if $z = -z_{sat}$, the synthesis is given by Fig.1.15. If $-z_{sat} < z < z_{sat}$, we have first a $\sigma_+\sigma_-$'s policy, then we encounter the case $u_s(z) = 3$ (see Fig.1.7), then we have a cut for $z > z_{sat}$.

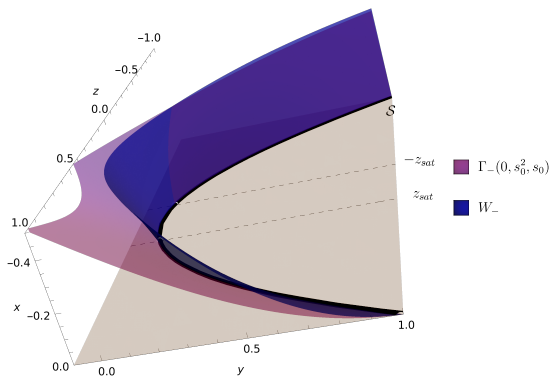
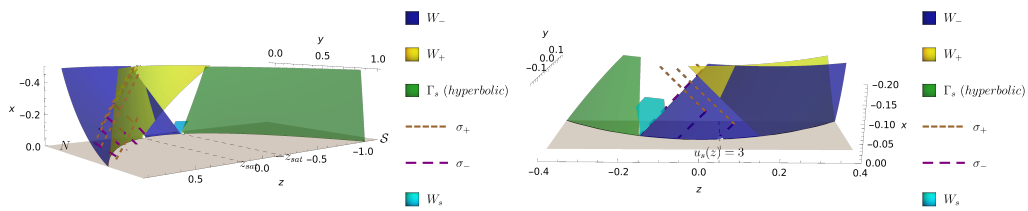


Fig. 1.17. The trajectories σ_- starting from $q_0 = (0, w_0, s_0)$ such that $w_0 > s_0^2$ switch on W_- for $z \in]-z_{sat}, 1[$ $(a = c = 1)$.



Cut locus for $z > z_{sat}$. $u_s(z) = 3$.

Fig. 1.18. *(left)* σ_- reflect on W_- for $z > z_{sat}$. *(right)* At $z = \frac{a}{18c} < z_{sat}$ such that $u_s(z) = 3$, σ_- cross W_- and the cut locus disappears (see Fig.1.7). For $-z_{sat} < z < z_{sat}$, the optimal policy is $\sigma_+\sigma_-$. The case $z = -z_{sat}$ was given in Fig.1.15 and is also represented here with the surface W_s.

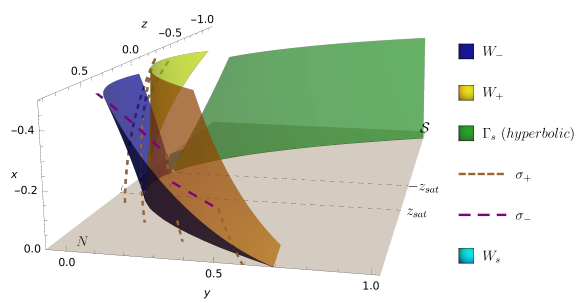


Fig. 1.19. For $z > z_{sat}$ σ_+ reflect on W_+, hence we have a cut locus. For $z < -z_{sat}$, the optimal policy is Bang-Singular.

Construction of a semi–normal form and the need of integrability assumption.

Notations and assumption: We normalize in a small neighborhood of N. We assume that F is transverse to N. Let $q = (x, y, z)$, $q_0 = (0, 0, 0)$, $G = \frac{\partial}{\partial z}$ and $N := \{x = 0\}$. We denote by σ_0 the reference trajectory of F identified to $t \to (t, 0, 0)$ so that $F_{|\sigma_0} = \frac{\partial}{\partial x}$.

Assuming x small enough one can write the system as:

$$\begin{aligned}\dot{x} &= 1 + f(y, z) + R_1\\ \dot{y} &= g(y, z) + R_2\\ \dot{z} &= h(y, z) + R_3,\end{aligned}$$

where $R_i(x, y, z) = o(|x|)$ and the corresponding model is

$$\begin{aligned}\dot{x} &= 1 + f(y, z)\\ \dot{y} &= g(y, z)\\ \dot{z} &= h(y, z) + u.\end{aligned}$$

Singular flow on the model: Furthermore, we assume $\frac{\partial g}{\partial z} \neq 0$. Since the singular flow is feedback invariant, setting $z = g(y, z)$, $z \to z$ and using a proper feedback the system takes the form

$$\begin{aligned}\dot{x} &= 1 + f(y, z)\\ \dot{y} &= z\\ \dot{z} &= u.\end{aligned}$$

Computing, we get:

$$\begin{aligned}&[G, F] = -f_z \frac{\partial}{\partial x} + \frac{\partial}{\partial y} \qquad [[G, F], G] = -f_{z^2} \frac{\partial}{\partial x},\\ &[[G, F], F] = -f_{yz} \frac{\partial}{\partial x} + f_y \frac{\partial}{\partial y}.\end{aligned} \tag{1.17}$$

Hence

$$D = -f_{z^2}, \qquad D' = -f_y f_z + f_{yz}$$

and

$$u_s = -\frac{D'}{D} = \frac{f_y f_z - f_{yz}}{f_{z^2}}.$$

Therefore, we have

$$\frac{\mathrm{d}y}{\mathrm{d}z} = \frac{z}{u_s}$$

and assuming the *separability condition*

$$\frac{\mathrm{d}y}{\mathrm{d}z} = h_1(y) h_2(z)$$

one can integrate the singular trajectories such that $q(0) \in \mathcal{S}$ as follows, parameterizing by z instead of t using the relation

$$\int_{y(0)}^{y} h_1(y)\,\mathrm{d}y = \int_{z(0)}^{z} h_2(z)\,\mathrm{d}z.$$

Assuming that $y(0)$ can be expressed as $y(0) = p_1(z(0))$ and moreover that the left–hand side is invertible, one gets $y = p_2(z, z(0))$. This defines the *singular leaf* $\mathcal{F}$ through $q(0) \in \mathcal{S}$ using the equation

$$\frac{\mathrm{d}x}{\mathrm{d}z} = \frac{1 + f(y, z)}{z}.$$

Using $x(0) = 0$, one gets:

$$x(z, z(0)) = \int_{z(0)}^{z} (1 + f(p_2(z, z(0)), z))\ \mathrm{d}z.$$

Remark 2. This requires an integrability condition to obtain the leaf $\mathcal{F}$. If it is not satisfied, integration is obtained through a proper *numeric integration.*

Application.

Singular set. Back to the tutorial model (1.16), we fix $a = c = 1$, we are in the separable case and using our previous algorithm one gets

Proposition 6. *1. Integrating the singular flow, we get:*

$$\begin{aligned} x(t, z(0)) &= t + \frac{2\varepsilon(2a+3ck)\left(kt+z(0)^2\right)^{5/2} - 10c\left(kt+z(0)^2\right)^3 t}{15k^2} \\ y(t, z(0)) &= \tfrac{2\varepsilon}{3k}\left(kt + z(0)^2\right)^{3/2} \\ z(t, z(0)) &= \varepsilon\left(kt + z(0)^2\right)^{1/2}, \end{aligned}$$

where $\varepsilon = \pm 1$, $k = 12c/a$.

2. Parameterizing by z*, the integral singular leaf* $\mathcal{F}$ *with* $q(0) \in \mathcal{S}$ *is given*

$$\begin{aligned} y(z, z(0)) &= 2c\,(z^3 - z(0)^3)/a + z(0)^2 \\ x(z, z(0)) &= g(z) - g(z(0)), \end{aligned}$$

where $g(z) = \dfrac{3cz^2}{5a^2}\Big(2a(2c+1)\,z^3 + 30cz(0)^2(a - 2cz(0))\,z + 30c^2\,z^4 + 5a(az(0)^2 - 2cz(0)^3 + 1)\Big)$.

We represent on Fig.1.20 the stratification of the singular leaf $\mathcal{F}$ with $a = c = 1$ using hyperbolic and elliptic cases and the admissibility conditions $|u_s| \leq 1$.

4.2 The 2d–McKeithan scheme

Recall that the network is $\begin{tikzcd} T + M \arrow[r, bend left, "k_1"] & A \arrow[l, bend left] \arrow[r, "k_2"] & B \arrow[ll, bend left, "k_3"] \arrow[lll, bend left, "k_4"] \end{tikzcd}$ 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 $T + M + A = \delta_1$ and $T + M + B = \delta_2$ takes the form

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

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

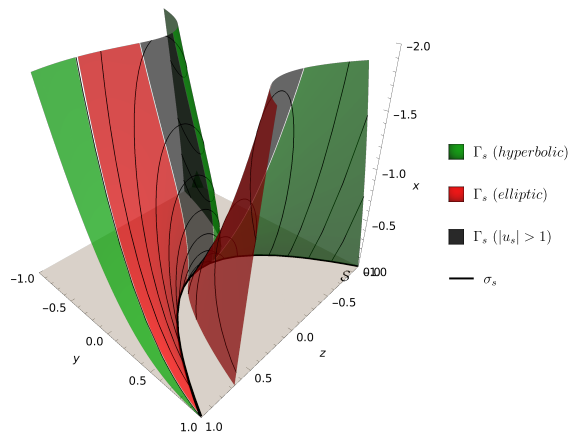


Fig. 1.20. Stratification of the singular set Γ_s for the system (1.16) with parameters $a = c = 1$.

4.2.1 Lie brackets computations

We have:

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

4.2.2 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: $u_s = -D'(q)/D(q)$.

4.2.3 Classification of local syntheses for the McKeithan network

We consider the case max $[A]$, with $x = [A]$. We proceed as follows.

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:

$$\begin{aligned} \mathcal{S} :\ \alpha_2\beta_2 d v^{\alpha_2 - 1} + \alpha_3\beta_3 d v^{\alpha_3 - 1} + d\delta_3 - \delta_4 \\ - d^2 + y(\delta_3 - 2d) - y^2 = 0. \end{aligned} \tag{1.18}$$

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

One has

Lemma 4. *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 9. *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

$$v^{\alpha_3 - \alpha_2} = -\frac{(\alpha_2 - 1)\alpha_2\beta_2}{(\alpha_3 - 1)\alpha_3\beta_3}. \tag{1.19}$$

Exceptional locus

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

$$\begin{aligned} \mathcal{E} :\ -\beta_2 d v^{\alpha_2} - \beta_3 d v^{\alpha_3} + d^2 v - d\delta_3 v \\ + y\,(2dv - \delta_3 v) + \delta_4 v + vy^2 = 0. \end{aligned} \tag{1.20}$$

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.1.21 gives a picture of stratification of $x = d$ for the McKeithan system with a focus where $\mathcal{S}$ is folded. We represent the sets $\mathcal{S}$ and $\mathcal{E}$ and the stratification of $\mathcal{S}$ in hyperbolic, elliptic and parabolic points. From this, we deduce the admissible points. We are in the flat case and a point of N is either an ordinary point or a fold point. For an ordinary point, the final optimal control is regular and is equal to $-\text{sign}\ \Phi(0)$. At a fold point on $\mathcal{S}$, the final optimal control may be singular (see Definition 7).

The optimal syntheses near the fold can be described using the techniques of the tutorial model (1.16) and symbolic computations.

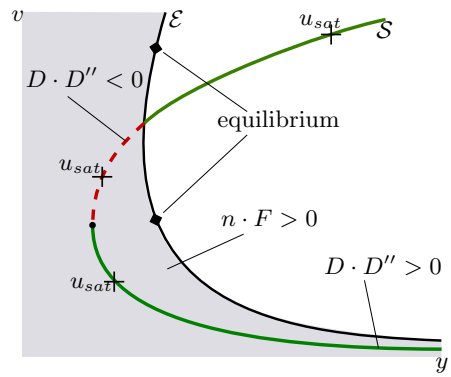


Fig. 1.21. Stratification of the surface $x = d$ for the McKeithan reaction. Dotted line: elliptic, red line: hyperbolic.

5 Conclusion

In this article, we have presented the general tools to analyze a Mayer problem to optimize the yield of chemical networks. Using the McKeithan network, we have completed the analysis of [8] for the simple scheme $A \to B \to C$.

The main point is to extend a geometric techniques from [9] to consider the case when the strict Legendre-Clebsch is not satisfied. The starting point is to analyze the semi-bridge phenomenon.

Note that with the same techniques we can analyze the situations up to codimension 2 describe in details in [21] (in particular near the exceptional locus $\mathcal{E}$). Furthermore, it can be extended to an important problem of codimension 3 occurring for reversible chemical networks and the existence of equilibria, see Fig. 1.21.

6 Appendix

6.1 Strata.m

```
(* Strata.m -- Tested with Mathematica v11.3 Linux *)
(*
This program computes the singular set, switching surface \
and splitting locus to derive the time minimal synthesis in a
    neighborhood of N.
*)
(* Lie derivative of w wrt v *)
LieDerive[v_List,w_List,var_List]:=Transpose[D[w,#]& /@ var] . v /; \
   Length[v] == Length[var]

(* Lie bracket [v,w] *)
LieBracket[v_List,w_List,var_List]:=\
   LieDerive[w,v,var] - LieDerive[v,w,var] /; \
```

```
  Length[v] == Length[w] == Length[var]

(* Poisson bracket {f,g} *)
PoissonBracket[f_, g_,q_List,p_List] /; Length[q] == Length[p] := \
  Total @ Flatten @ Fold[List,0,MapThread[D[f,#1] D[g,#2] - D[f,#2]
      D[g,#1] &, {q, p}]]

(* Remove monomials of order >= ord *)
EliminTe[expr_,var_List,ord_Integer]:=Module[{},\
  FromCoefficientRules[Select[CoefficientRules[expr,var],Total@#[[1]]
      <= ord &], var]]

(* Multivariate Taylor expansions *)
mTaylor[expr_,var_List,pts_List,ord_Integer] /; \
  Length[var] == Length[pts] := Normal[Series[(expr /. Thread[var ->
      s (var - pts) + pts])//ExpandAll, {s, 0, ord}]] /. {s -> 1}

(*
  Integration in (q,p) of H=p.(XX + u YY) for small time in o(t^ord)
*)
IntSmallTime[XX_,YY_,u_,qfpf_List,ord_Integer]:=Module[{res},
 pv        = {p1,p2,p3};
 qv        = {x,y,z};
 H         = {p1,p2,p3}.(XX + u YY);
 res       = Sum[t^k / k!
     Nest[PoissonBracket[#,H,qv,pv]&,#,k],{k,0,ord}] \
             /. Thread[Join[qv,pv]->qfpf]& /@ Join[qv,pv]
];


$Assumptions = (ep==1 || ep==-1);

(*-------------------------------------------------------*)
(*-------------------------main--------------------------*)
(*-------------------------------------------------------*)

(*.......... constants ..........*)
a1        = 1;     a2 = 1;     a4 = 1;
b         = 1;      c = 1;      d = 0;
uh0       = 1;     uhx = 1;   uhy = 1;

(*.......... model ..........*)
XX        = {1 + a z^2 + a2 x z^2 + a3 x y^2 + a4 y z^2,\
          b z, -uh0 -uhx x -uhy y + c z};
X         = XX /. {x-> x-d};
Y         = {0,0,1};

(*.......... Lie brackets computations ..........*)
YX        = LieBracket[Y,X,{x,y,v}];
```

```
YXY         = LieBracket[YX,Y,{x,y,v}];
YXX         = LieBracket[YX,X,{x,y,v}];
DD          = Det[{Y,YX,YXY}];
DDp         = Det[{Y,YX,YXX}];
DDpp        = Det[{Y,YX,X}];
aux         = Solve[(YX[[1]])==0,{y}];
Sy[v_]      = Expand[(y /. aux[[1]]) /. x->0]

(*.......... Gammas ..........*)
ord         = 3;
us          = - DDp / DD;
q0p0        = {0,w0,0,1,0,0};
qpt         = IntSmallTime[X,Y,us,q0p0,ord];
ps          = {t0val,w0val,s0val};
gms         = mTaylor[#,{t,w0,s0},ps,ordG]& /@ qpt[[1;;3]] //Expand
gmsall      = mTaylor[#,{t,w0,s0},ps,ordG]& /@ qpt //Expand

(*.......... Gamma+,Gamma- ..........*)
u           = ep;
q0p0        = {0,w0,s0,1,0,0};
pt          = {t0val,w0val,s0val};
qpt         = Refine /@ IntSmallTime[X,Y,u,q0p0,ord];
qpt         = mTaylor[#,{t,w0,s0},pt,ordG] & /@ qpt;
gmall       = Refine /@ qpt //Refine
gmp         = gmall[[1;;3]] /. {ep->1}
gmm         = gmall[[1;;3]] /. {ep->-1}


(*.......... W+,W- ..........*)
ord         = 3;
qpt         = Refine /@ IntSmallTime[X,Y,u,q0p0,ord];
eq          = mTaylor[qpt[[6]],vars,{t0val,w0val,s0val},ord] // Simplify
aux         = Solve[eq==0,vw];
sols        = Flatten[vw /. aux];
sols        = Refine[Expand[mTaylor[#,{t,w0,s0},{0,w0val,s0val},ord] &
    /@ sols]] // Simplify
solp        = mTaylor[ # /. {ep->1},vars,{t0val,w0val,s0val},ordG] & /@
    sols;
solm        = mTaylor[ # /.{ep->-1},vars,{t0val,w0val,s0val},ordG] & /@
    sols
qptp        = (qpt /. ep->1 /. vw-># ) & /@ solp;
qpwps       = mTaylor[#,{t,w0,s0},pt,ordG] & /@ qptp // Flatten;
qptm        = (qpt /. ep->-1 /. vw-># ) & /@ solm;
qpwms       = mTaylor[#,{t,w0,s0},pt,ordG] & /@ qptm //Flatten

(*.......... Ws ..........*)
ord         = 3;
q0p0        = {0,w0,0,1,0,0};
qpt         = Refine /@ IntSmallTime[X,Y,us,q0p0,ord];
```

```
qpt        = mTaylor[#,{t,w0,s0},pt,ord] & /@ qpt;
q0p02      = qpt /. t->ss;
qpt2       = Refine /@ IntSmallTime[X,Y,1,q0p02,ord];
qpt2       = mTaylor[#,{t,w0,s0,ss},{0,w0val,s0val,0},ord] & /@ qpt2;
p3t2       = qpt2[[6]]
aux        = Solve[p3t2==0,ss];
sols       = Flatten[ss /. aux];
sols       = Refine[Expand[mTaylor[#,{t,w0,s0},{0,w0val,s0val},ord] &
    /@ sols]]
qpws       = qpt2 /. {ss-> #} & /@ sols;
qpws       = mTaylor[#,{t,w0,s0},pt,ordG] & /@ qpws //Flatten
ws         = Refine /@ qpws[[1;;3]]

(*.......... C1 ..........*)
ord        = 3;
q0p0       = {0,w0,s0,1,0,0};
pt         = {0,w0val,s0val};
qpt        = IntSmallTime[X,Y,u,q0p0,ord];
qpt        = mTaylor[#,{t,w0,s0},pt,ord] & /@ qpt;
(* u=-1 *)
{xp,yp,zp} = qpt[[1;;3]] /.{ep->-1};
(* u=+1 *)
{xm,ym,zm} = qpt[[1;;3]] /.{ep->1,s0->s0p,w0->w0p};

eqns       = {xp==xm,yp==ym,zp==zm};
aux        = Solve[eqns,{t,w0p,s0p}] // Expand;
aux2       = {t,w0p,s0p} /. aux;
c1sols     = mTaylor[#,{t,w0,s0},pt,ord] & /@ aux2;

(*.......... C12 ..........*)
ord        = 2;
q0p0       = {0,w0,s0,1,0,0};
pt         = {0,w0val,s0val};
qpt        = IntSmallTime[X,Y,u,q0p0,ord];
qpt        = mTaylor[#,{t,w0,s0},pt,ord] & /@ qpt;
vars       = {t,ss1,ss2,w0,s0,w0p,s0p};
pt2        = {0,0,0,w0val,s0val,w0val,s0val};

(* u=-1 *)
{x1,y1,z1} = qpt[[1;;3]] /.{ep->-1};

(* u=-1 & switch *)
ptfin      = (qpt /.{ep->-1,w0->w0p,s0->s0p})/.t->ss1;
qpt2       = IntSmallTime[X,Y,1,ptfin,ord] /. t->ss2;
{x3,y3,z3} = mTaylor[#,vars,pt2,ord] & /@ qpt2[[1;;3]];

eqns       = {x1==x3,y1==y3,z1==z3,ss2+ss1==t,ptfin[[6]]==0};
aux        = Solve[eqns,{t,ss1,ss2,w0p,s0p}];
aux2       = {t,ss1,ss2,w0p,s0p} /. aux;
```

```
c12sols    = mTaylor[#,vars,pt2,ord] & /@ sols;
```

References

1. A. Agrachev , R.V. Gamkrelidze, *Symplectic methods for optimization and control*, in Geometry of Feedback and Optimal Control, Monogr. Textbooks Pure Appl. Math. **207**, B. Jakubczyk and W. Respondek, eds., Marcel Dekker, New York, (1998) pp. 19–77
2. D. Anderson, *Global asymptotic stability for a class of nonlinear chemical equations*, SIAM J. Appl. Math. **5** no.68 (2008) 1464–1476.
3. V.G. Boltyanskii, *Sufficient conditions for optimality and the justification of the dynamic programming method*, SIAM J. Control Optim., **4** (1966) 326–361.
4. B. Bonnard, *Feedback equivalence for nonlinear systems and the time optimal control problem*, SIAM J. Control Optim. **29**, no.6, (1991) 1300–1321.
5. B. Bonnard, M. Chyba, *Singular trajectories and their role in control theory*, Mathématiques & Applications **40** Springer-Verlag Berlin Heidelberg, 2003 xvi+357.
6. B. Bonnard, O. Cots, J. Rouot, T. Verron, *Time minimal saturation of a pair of spins and application in magnetic resonance imaging*, Math. Control Relat. Fields, AIMS (2019).
7. B. Bonnard, I. Kupka, *Théorie des singularités de l'application entrée/sortie et optimalité des trajectoires singulières dans le problème du temps minimal*, Forum Math. **5**, no.2 111–159 (1993).
8. B. Bonnard, G. Launay, *Time minimal control of batch reactors*, ESAIM: Control, Optimisation and Calculus of Variations **3** (1998) 407–467.
9. B. Bonnard, G. Launay, M. Pelletier, *Classification générique de synthèses temps minimales avec cible de codimension un et applications*, Annales de l'I.H.P. Analyse non linéaire **14** no.1 (1997) 55–102.
10. B. Bonnard, M. Pelletier, *Time minimal synthesis for planar systems in the neighborhood of a terminal manifold of codimension one*, J. of Mathematical Systems, Estimation and Control **5** no.3 (1995) 379–381.
11. B. Bonnard, D. Sugny, *Optimal Control with Applications in Space and Quantum Dynamics*, AIMS Series on Applied Mathematics **5**, 2012 xvii+298.
12. U. Boscain, B. Piccoli, *Optimal Syntheses for Control Systems on 2-D Manifolds*, Mathématiques et Applications, **43** Springer–Verlag Berlin Heidelberg, 2004 xiv–262.
13. P. Brunovsky, *Existence of Regular Syntheses for General Problems*, J. Diff. Equations **38** (1980) 317–343.
14. M. Chavez, *Observer design for a class of nonlinear systems, with applications to chemical and biological networks*, Ph.D. thesis, Rutgers University, New Brunswick, NJ, 2003.
15. M. Chavez, E. Sontag, *State-estimators for chemical reaction networks of Feinberg–Horn–Jackson zero deficiency type*, Euro. J. Cont. **8** (2002) 343–359.
16. I. Ekeland, *Discontinuité des champs hamiltoniens et existence des solutions optimales en calcul des variations*, Inst. Hautes Études Sci. Publ. Math. **47**, (1977) 5–32.

17. M. Feinberg, *On chemical kinetics of a certain class*, Rational Mech. Anal., **46** no.1, (1972).
18. F. Horn, R. Jackson, *General mass action kinetics*, Arch. Ration. Mech. Anal., **47** no.1, (1972) 81–116.
19. A. J. Krener, *The high order maximal principle and its application to singular extremals.* SIAM Journal on Control and Optimization, **15** no.2, (1977) 256–293.
20. I. Kupka, *Geometric theory of extremals in optimal control problems. I. The fold and Maxwell case*, Trans. Amer. Math. Soc. **299** no.1, (1987) 225–243.
21. G. Launay, M. Pelletier, *The generic local structure of time-optimal synthesis with a target of codimension one in dimension greater than two.* J. Dynam. Control Systems **3** no.2 (1997) 165–203.
22. J. Martinet, *Singularities of smooth functions and maps*, London Mathematical Society Lecture Note Series, **58**, Cambridge University Press, Cambridge-New York, 1982, xiv+256.
23. T.W. McKeithan *Kinetic proofreading in T-cell receptor signal transduction* Proc. Natl. Acad. Sci. USA, **92** (1995) 5042–5046.
24. L.S. Pontryagin, V.G. Boltyanskii, R.V. Gamkrelidze, E.F. Mishchenko, *The mathematical theory of optimal processes*, Oxford, Pergamon Press, 1964.
25. H. Schättler, U. Ledzewicz, *Geometric optimal control. Theory, methods and examples*, Interdisciplinary Applied Mathematics, **38** Springer-Verlag New York, 2012 xx+640.
26. H. Schättler, *On the local structure of time-optimal bang-bang trajectories in* R^3, SIAM J.Control Optim., **26** (1988) 186–204.
27. E.D. Sontag *Structure and stability of certain chemical networks and applications to the kinetic proofreading model of T-cell receptor signal transduction* IEEE Trans. Automat. Contr. **46** no.7 (2001) 1028–1047.
28. H.J. Sussmann, *Synthesis, presynthesis, sufficient conditions for optimality and subanalytic sets*, Nonlinear Controllability and Optimal Control, H.J. Sussmann Ed., Marcel Dekker, New York, (1990) 1–20.
29. H.J. Sussmann, *The Structure of Time–Optimal Trajectories for Single–Input Systems in the Plane: the* $\mathcal{C}^\infty$ *Nonsingular Case*, SIAM J. Control and Opt. **25** (1987) 433–465.
30. H.J. Sussmann, *The Structure of Time–Optimal Trajectories for Single–Input Systems in the Plane: the General Real Analytic case*, SIAM J. Control and Opt. **25** (1987) 868–904.
31. J. Tóth, A. L. Nagy, D. Papp, *Reaction kinetics: exercises, programs and theorems*, Springer-Verlag New York, 2018 xxiv+469.
32. E. Trélat, E. Zuazua, *The turnpike property in finite-dimensional nonlinear optimal control*, J. Differential Equations, **258** (2015) 81–114.