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Time Minimal Syntheses in the Exceptional Case using Geometric and Computational Techniques.

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Abstract: This article deals with the optimization of chemical network in the frame of geometric optimal control and singularity theory. The objective is to classify the generic syntheses for analytic systems of the form $\dot{q}(t) = X(q(t)) + u(t)Y(q(t))$, where the aim is to reach in minimum time a terminal manifold of codimension one. We develop symbolic algorithms to compute approximations of the strata of the singular set to derive the topological classification in the generic cases and to illustrate the role of singularity theory in geometric control, in relation with abnormal geodesics and regularity of the value function, solution of Hamilton-Jacobi-Bellman equation.

Keywords: Chemical reaction networks · Geometric optimal control · Time minimal syntheses · Regularity of the value function

INTRODUCTION

Within the last decades, reactors dynamics has been an important research area [Feinberg, 1972, Horn et al, 1972], having some industrial impact where the control of such processes is a substantial task. One important application in medicine concerns the control of the McKeithan network [McKeithan, 1995] aiming to maximize the production of one species, e.g. A . Assuming that the dependence with respect to the ambient temperature is described by the Arrhenius law, and using the derivative of the temperature as a control, which consists into Goh transformation, the problem can be transformed into a time minimal control problem with a $3d$ -affine system and where the terminal manifold N is given by fixing at the final time a fixed amount of the desired species [Bonnard et al, 2019]. Such process can be modeled by a system in \mathbb{R}^3 of the form

$$\dot{q}(t) = X(q(t)) + u(t)Y(q(t)), \quad |u| \leq 1, \quad (1)$$

where X, Y are analytic vector fields, the control $u(\cdot)$ is a measurable function on $[0, T]$ and we require that $q(T) \in N$.

In this context, among a series of works, the article [Bonnard et al, 1997] addressed the problem of computing in a neighborhood of N the feedback optimal control $u^*(q)$, which reaches N from q in minimum time. The techniques combine tools from singularity theory adapted to control theory to determine the time minimal syntheses using the concept of graded semi-normal forms and unfolding [Arnol'd, 1991]. The aim of this article is to complete the results of [Bonnard et al, 1997, Launay et al, 1997]

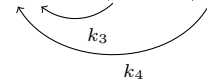
in the so-called abnormal (or exceptional) case where the geodesics are tangent to the terminal manifold N .

The singularity theoretical frame was already present in those earliest references: construction of semi-normal form and concept of unfolding but recent progress of formal languages are used to handle complicated computation in particular in relation with the (reversible) McKeithan network.

1. TIME MINIMAL EXCEPTIONAL GEODESICS IN OPTIMIZATION OF CHEMICAL NETWORKS

1.1 A brief recap about the optimal control of chemical networks

In this section, we introduce the concepts for the optimization of chemical networks. In particular we shall consider the McKeithan network: $T + M \xrightarrow{k_1} A \xrightarrow{k_2} B$.



The state space is formed by the concentration vector:

$$c = (c_T, c_M, c_A, c_B)$$

of the respective chemical species. We note $\delta_1 = c_T + c_A + c_B$, $\delta_2 = c_M + c_A + c_B$ the first integrals associated to the dynamics and let $x = c_A$, $y = c_B$, then the system is described by the equation:

$$\begin{aligned} \dot{x} &= -\beta_2 x v^{\alpha_2} - \beta_3 x v^{\alpha_3} - \delta_3 v (x + y) + \delta_4 v + v (x + y)^2 \\ \dot{y} &= \beta_2 x v^{\alpha_2} - \beta_4 y v^{\alpha_4} \\ \dot{z} &= u, \quad |u| \leq 1, \end{aligned}$$

with

* The authors thank Bernard Bonnard for the fruitful discussions.

$0 \leq x \leq \delta_1$, $0 \leq y \leq \delta_2$, $\delta_3 = \delta_1 + \delta_2$, $\delta_4 = \delta_1 \delta_2$,
the Arrhenius law gives $k_i = A \exp(-E_i/RT)$, $i = 1, 2, 3, 4$
(E_i is the activation energy, T is the temperature, A, R are
constant) and

$$z = k_1, k_2 = \beta_2 v^{\alpha_2}, k_3 = \beta_3 v^{\alpha_3}, k_4 = \beta_4 v^{\alpha_4}.$$

Maximizing the product of the A species leads to a time
minimal control problem with a terminal manifold $N : x =$
 d , d being the desired production of A , see [Bonnard et al,
2019] for more details.

We denote by $\dot{q} = X + uY$, $|u| \leq 1$ the control system.

1.2 Time minimal control for 3d-affine systems and Maximum Principle

We consider a three dimensional single-input control sys-
tem of the form

$$\frac{dq}{dt}(t) = X(q(t)) + u(t)Y(q(t))$$

with $q = (x, y, z)$, (X, Y) being smooth (C^∞ or C^ω) vector
fields and the control $u(\cdot)$ is a measurable mapping on
 $J = [0, t_f(u)]$ valued in the interval $[-1, +1]$. We denote
by $q(\cdot, q_0, u)$ the response to $u(\cdot)$ defined on a subinterval
of J , with $q(0) = q_0$, written in short as $q(\cdot)$. Together
with this controlled dynamics, our aim is to minimize the
time to reach a terminal manifold N of codimension 1.

Maximum principle [Pontryagin et al, 1964]. Con-
sider the problem of optimizing the transfer time from q_0 to
a smooth submanifold N of \mathbb{R}^3 . Then, if the pair $(u(\cdot), q(\cdot))$
is optimal on $[0, t_f]$ there exists an absolutely continuous
vector function $p(\cdot)$ such that the following conditions are
satisfied. Denoting $H(q, p, u) = p \cdot (X + uY)$, with \cdot the
scalar product of \mathbb{R}^3 , one has:

- (1) the triplet (q, p, u) is solution a.e. on $[0, t_f]$ of

$$\begin{aligned} \dot{q} &= \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}, \\ H(q, p, u) &= \max_{|v| \leq 1} H(q, p, v). \end{aligned} \quad (2)$$

- (2) $M(q, p) = \max_{|v| \leq 1} H(q, p, v)$ is constant and equals
to $-p_0$ and $-p_0$ is nonnegative in the time minimal
case and nonpositive in the time maximal case.
(3) The vector $p(\cdot)$ satisfies at the final time t_f the
transversality conditions

$$p(t_f) \perp T_{q(t_f)}N.$$

Definition 1. A triplet (q, p, u) solutions of (2) is called
an extremal and the q -projection is called a geodesic. If
moreover it satisfies the transversality condition it is called
a BC-extremal. An extremal is called regular if the control
is given by $u(t) = \text{sign } p(t) \cdot Y(q(t))$ a.e.. It is called bang-
bang if the number of switches is finite. An extremal is
called singular if $p(t) \cdot Y(q(t)) = 0$ on $[0, t_f]$. An extremal
is called abnormal (or exceptional) if $p_0 = 0$, so that it is
candidate to minimize or maximize the transfer time.

Computation of the singular controls. If z_1, z_2 de-
note two (smooth) vector fields, the Lie bracket is com-
puted with the convention:

$$[Z_1, Z_2](q) = \frac{\partial Z_1}{\partial q}(q)Z_2(q) - \frac{\partial Z_2}{\partial q}(q)Z_1(q).$$

In the singular case, deriving twice the equation $t \mapsto p(t) \cdot$
 $Y(q(t)) = 0$, one gets:

$$\begin{aligned} p(t) \cdot Y(q(t)) &= p(t) \cdot [Y, X](q(t)) = 0, \\ p(t) \cdot ([Y, X], X)(q(t)) + u(t)[Y, X], Y(q(t)) &= 0. \end{aligned}$$

Introducing the determinants:

$$\begin{aligned} D &= \det(Y, [Y, X], [[Y, X], Y]), \\ D' &= \det(Y, [Y, X], [[Y, X], X]), \\ D'' &= \det(Y, [Y, X], X), \end{aligned}$$

one has the following.

Proposition 2. If D is nonzero, the singular controls are
defined by the feedback $u_s(q) = -D'(q)/D(q)$ so that
the corresponding geodesics are solutions of the vector
field : $X_s(q) = X(q) + u_s(q)Y(q)$. Abnormal (exceptional)
geodesics are contained in the set $D'' = 0$.

**High-order Maximum Principle in the singular
case.** To distinguish between time minimizing or max-
imizing geodesics, one needs to use the high-order Maxi-
mum Principle, see [Krener, 1977].

Proposition 3. Candidates to time minimizing are con-
tained in $DD'' \geq 0$ and candidates to time maximizing
are contained in the set $DD'' \leq 0$. If the corresponding in-
equalities are strict, they are respectively called hyperbolic
or elliptic.

2. TIME MINIMAL SYNTHESIS IN THE EXCEPTIONAL CASES

2.1 General concepts and notation

We consider a local neighborhood U of $q_0 \in N$, which can
be identified to 0. One wants to describe the time minimal
syntheses in a small neighborhood U of 0. We denote
respectively by σ_\pm^0 , σ_s^0 bang and singular arcs terminating
at 0 and we consider only the exceptional case, where the
arc is tangent to N and splits into the bang exceptional
case or the singular exceptional case.

In U , each optimal solution is a concatenation by arcs
 σ_+, σ_- , where the control is $u = \pm 1$ and singular arcs
 σ_s . Our method consists of the construction of *semi-*
normal forms for the action of the pseudo-group \mathcal{G} of local
diffeomorphisms φ such that $\varphi(0) = 0$, $\varphi * Y = Y$ and
feedback transformation $u \rightarrow -u$ (so that σ_+ and σ_-
can be exchanged).

If the optimal control $u^*(v) \in [-1, 1]$ exists and is unique,
it is regular on an open subset of U , union of U_+ where
 $u^*(v) = 1$ and U_- where $u^*(v) = -1$. The surface S which
separates U_+ from U_- is subanalytic and can be stratified
into [Boltyanskii, 1966]

- a switching locus W : closure of the set of points where
 u^* is regular and not continuous. We denote by W_+
(resp. W_-) the points of W where the optimal control
is $+1$ (resp. -1) on N ,
- a cut-locus C : closure of the set of points where a
trajectory loses its (global) optimality,
- singular locus Γ_s : union of optimal singular trajecto-
ries,

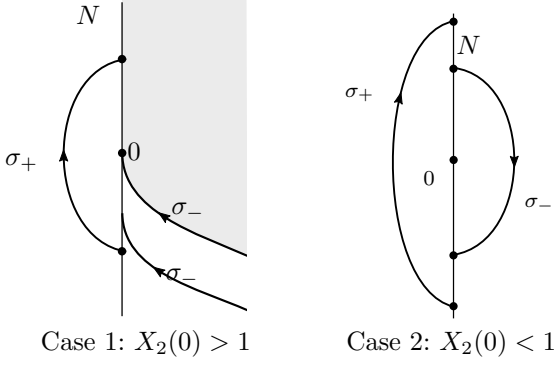


Fig. 1. Local synthesis near \mathcal{E} in the generic case.

and these strata can be approximated by semialgebraic sets using seminormal forms.

The syntheses are described in details in [Bonnard et al, 1997, Launay et al, 1997] up to the codimension two situations and we recall below the main points to be applied to the McKeithan network.

2.2 Local syntheses in the exceptional cases

The bang exceptional case. In the bang exceptional situation, we have to consider the two following cases.

Generic case (codimension one). In this case both arcs σ_+ and σ_- arc tangent to N but with a contact of order 2. Using the concept of unfolding, one can define a C^0 -foliation of U by invariant planes so that in each plane the system takes the semi-normal form:

$$\begin{cases} \dot{x} = by + o(|x|, |y|) \\ \dot{y} = X_2(x, y) + u, \quad |u| \leq 1, \end{cases} \quad (3)$$

where $b = n \cdot [Y, X] \neq 0$, which can be normalized to 1, $n = (1, 0)$ being the normal to N identified to $x = 0$. Moreover one can assume that $1 + X_2(0) > 0$ and we have two cases.

Proposition 4. Using the previous normalization we have two cases described in Fig.1.

The difference between the two cases is related to different accessibility properties of the system. In the case $X_2(0) > 1$, the target N is not accessible from the points in $x > 0$ above the arc σ_-^0 terminating at 0 . In the case $X_2(0) < 1$, each point of U can be steered in minimum time to N , the domain U_+ where the optimal control is $+1$ being $x < 0$ and the domain U_- with optimal control -1 being $x > 0$.

Codimension two case. A more complex situation occurs assuming that the arc σ_-^0 has a contact of order three with N , while σ_+^0 has a contact of order two. The optimal syntheses cannot be described by foliating N by $2d$ -planes as in the previous cases.

One needs to introduce the following assumptions. We assume that $Y = \frac{\partial}{\partial z}$, N is the plane $x = 0$ parameterized as the image of: $(w, s) \mapsto (0, w, s)$. Denoting $n = (1, 0, 0)$, the normal to N at 0 , we assume

- bang exceptional case: $n \cdot X(0) = 0$, $n \cdot [Y, X](0) \neq 0$,
- $\det(X, Y, [Y, X]) \neq 0$ at 0 ,
- $\{n \cdot X = 0\} \cap N$ is a curve which is neither tangent to X nor to Y at 0 .

We introduce the following normalization: along the y -axis, $n \cdot X = 0$ and $[X, Y] = \frac{\partial}{\partial x}$.

Using the concept of semi-normal form the optimal syntheses can be described by the following model:

$$\begin{cases} \dot{x} = z \\ \dot{y} = b, \\ \dot{z} = 1 + u + y \end{cases} \quad N : (w, s) \mapsto (0, w, s), \quad (4)$$

and we have two types of time minimal syntheses.

Proposition 5. Assume $b < 0$. Then each point of U can be steered to N . Moreover

- (1) $U^+ \setminus N \subset \{x < 0\}$ and $U^- \setminus N \subset \{x > 0\}$
- (2) Optimal trajectories σ_- arrive at any point $(0, w, s < 0)$ or $(0, w \geq 0, s)$ of $N \cap U$.

The optimal synthesis is described by Fig.2.

Proposition 6. Assume $b > 0$. In this case the system is not locally controllable at 0 . We represent on Fig.3 the synthesis in this case.

We shall refer to [Launay et al, 1997] for the full details of the computation and description of the syntheses.

The singular exceptional case. In this case we can assume $Y = \frac{\partial}{\partial z}$, N is the plane $x = 0$, the normal to N at 0 is $n = (1, 0, 0)$ and moreover:

$$\begin{cases} n \cdot X(0) = 0 \\ n \cdot [Y, X](0) = 0 \end{cases}$$

and we add the following generic conditions

- X and Y are independent at 0 ,
- $\det(Y, [Y, X], \text{ad}^2 Y \cdot X) \neq 0$ at 0 ,
- $\{n \cdot X = 0\} \cap N$ is a curve which is not tangent to X at 0 .

Using the concept of semi-normal form the optimal syntheses can be described by the following

$$\begin{cases} \dot{x} = y + z^2 \\ \dot{y} = b + b_1 z. \\ \dot{z} = c + u \end{cases} \quad (5)$$

In this model, the exceptional locus $\mathcal{E} \cap N$ is approximated by the parabola: $w + s^2 = 0$ and we denote by $\mathcal{E}_- : \{n \cdot X(q) < 0\} \cap N$ and $\mathcal{E}_+ = \{n \cdot X(q) > 0\} \cap N$.

We revise the six cases presented in [Launay et al, 1997], where we compute the optimal policies using symbolic computation (obtaining a different result for the Case 3). One noticeable difference with the non exceptional case (see [Bonnard et al, 1997]) is the presence of trajectories intersecting N twice and leads to an other component of S .

- *Case 1:* $b > 0$, $u_s(0) > 3$. The surface S is a union of the switching locus and a subset of \mathcal{E}_- .
- *Case 2:* $b > 0$, $1 < u_s(0) < 3$. The surface S is the union of a splitting locus, a switching locus and a subset of \mathcal{E}_- .
- *Case 3:* $b > 0$, $0 \leq u_s(0) < 1$. The surface S is the union of a singular locus filled by admissible singular

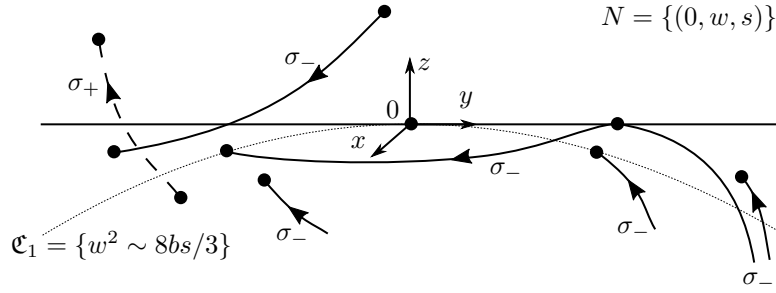


Fig. 2. Local synthesis near \mathcal{E} in the codimension 2 case for $b < 0$. The dashed curves are in the region $x \leq 0$.

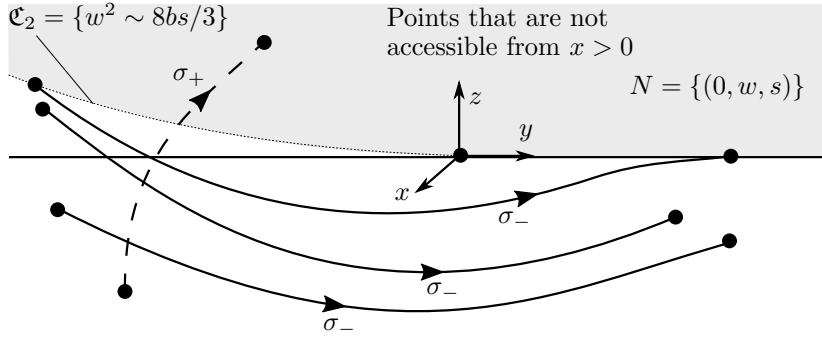


Fig. 3. Local synthesis near \mathcal{E} in the codimension 2 case for $b > 0$.

arcs, a splitting locus, a switching locus and a subset of \mathcal{E}_- .

- *Case 4:* $b < 0$, $u_s(0) > 3$. In this situation the set S is the union of a switching locus and a subset of \mathcal{E}_+ .
- *Case 5:* $b < 0$, $1 < u_s(0) < 3$. In this case S is the union of a splitting locus, a switching locus W_+ and a subset of \mathcal{E}_+ .
- *Case 6:* $b < 0$, $0 \leq u_s(0) < 1$. In this case S is a union of a singular locus, a splitting locus and \mathcal{E}_+ .

This gives the complete classification under generic assumptions. Again the stratification of S can be computed in the original coordinates and applied to the McKeithan network.

Illustration of the method based on symbolic computation. We present an algorithm to compute an approximation of the surface S in the codimension 2 case, more specifically we treat the Case 3 described above and given by the model (5) with $b > 0$ and such that the singular trajectory arriving at 0 is not saturating, that is $0 \leq b_1/2 - c < 1$.

Method. The following steps involve symbolic computation to obtain the optimal policy based on [Kupka, 1987].

1. Take $q(0) = (0, w, s) \in N \cap U$. We first determine the stratification of the surface N . Since Y is tangent to N , $q(0)$ is a switching point. If $q(0)$ is an ordinary switching point, the optimal control is regular: $u(0) = \text{sign}(p(0) \cdot [Y, X](0))$. If it is a fold point, the optimal control may be singular and the optimal policy is determined using [Bonnard et al., 1993]. Note that since $u_s(0) = b_1/2 - c < 1$,

the singular trajectories cannot be parabolic but either hyperbolic or elliptic, which corresponds respectively to time minimizing or time maximizing trajectories.

2. We then integrate the system backward in time from $q(0)$ and compute the equations characterizing the switching surface, the splitting locus C_s and the singular locus Γ_s .

A trajectory $\sigma_\varepsilon, \varepsilon \in \{-1, 1\}$ can switch at time $t_1^\varepsilon < 0$, can intersect the surface N at time $t_2^\varepsilon < 0$ or there may exist a time $t_3 < 0$ and a point $q_3 \in V$ such that $\exp(-t_3(X + Y))(q_3) = q(0)$, $\exp(-t_3(X - Y))(q_3) \in N$ and $t_3 < 0$.

The weights of the variable t, s, w is respectively 1, 2, 1. We develop the regular flow using Taylor expansion up to order 3 in t , we obtain :

$$\begin{aligned}
 p_3(t_1^\varepsilon) = 0 &\Rightarrow t_1^\varepsilon = \frac{2s}{b_1/2 - c - \varepsilon} + \dots, \\
 e^{t_2^\varepsilon(X + \varepsilon Y)}(q(0)) \in N &\Rightarrow t_2^\varepsilon = \frac{-2}{b} (w + s^2) + \dots, \\
 \exists (t_3, q) \in \mathbb{R}_*^- \times U, &\begin{cases} e^{-t_3(X + Y)}(q) \in N \\ e^{-t_3(X - Y)}(q) \in N \end{cases} \\
 &\Rightarrow t_3 = \frac{3s}{b_1/2 - c - 3} + \dots
 \end{aligned} \tag{6}$$

and a parameterization of

- the switching surface $W_- = (x(w, s), y(w, s), z(w, s))$ is

$$\begin{aligned}
x(w, s) &= \frac{s^2 (9b_1^2 - 4b_1(c + \varepsilon) + 4(c + \varepsilon)^2) + 3w(b_1 - 2(c + \varepsilon))^2}{3(b_1 - 2(c + \varepsilon))^3/4s} + \\
&\frac{6bs(b_1 - 2(c + \varepsilon))}{3(b_1 - 2(c + \varepsilon))^3/4s} + \dots, \\
y(w, s) &= \frac{4s (b(b_1 - 2(c + \varepsilon)) + b_1^2 s)}{(b_1 - 2(c + \varepsilon))^2} + w + \dots, \\
z(w, s) &= \frac{s(b_1 + 2(c + \varepsilon))}{b_1 - 2(c + \varepsilon)} + \dots,
\end{aligned} \tag{7}$$

- the singular surface $\Gamma_s := \Gamma_s(t, w)$ is

$$\Gamma_s = \left(\frac{bt^2}{2} + \frac{b_1^2 t^3}{6} + tw, bt + \frac{b_1^2 t^2}{4} + w, \frac{b_1 t}{2} \right) + \dots, \tag{8}$$

- and the splitting locus $C_s = (x(w, s), y(w, s), z(w, s))$ is

$$\begin{aligned}
x(w, s) &= \frac{2s^2 (b_1 c + b_1(2b_1 - 9) + 2c^2 + 6) + w(b_1 - 2c - 6)^2}{(b_1 - 2(c + 3))^3/6s} \\
&+ \frac{3bs(b_1 - 2(c + 3))}{(b_1 - 2(c + 3))^3/6s} + \dots, \\
y(w, s) &= \frac{6s(b(b_1 - 2(c + 3)) + b_1 s(b_1 + c - 3))}{(b_1 - 2(c + 3))^2} + w + \dots, \\
z(w, s) &= \frac{s(b_1 + 4c)}{b_1 - 2(c + 3)} + \dots
\end{aligned} \tag{9}$$

3. The optimal policy is deduced by computing $t^* = \max(t_1^\varepsilon, t_2^\varepsilon, t_3)$ with $\varepsilon = \text{sign}(s(n \cdot X(0, w, s)))$ and we represent in Fig.5 the region of N where $t^*(w, s)$ corresponds to a switching time, a splitting time or a time at which the trajectory intersects N . The surface S separating U_+ and U_- is the union of the switching surface W_- , the singular surface Γ_s foliated by singular arcs, the splitting locus C_s and a subset $\tilde{\mathcal{E}}_- \subset \mathcal{E}_-$ from which σ_\pm intersects N in the green region of Fig. 5. The set S is represented in Fig. 4 together with some trajectories emanating from N to the components of S . The green trajectories starting from \mathcal{E}_+ intersect N in $\tilde{\mathcal{E}}_-$.

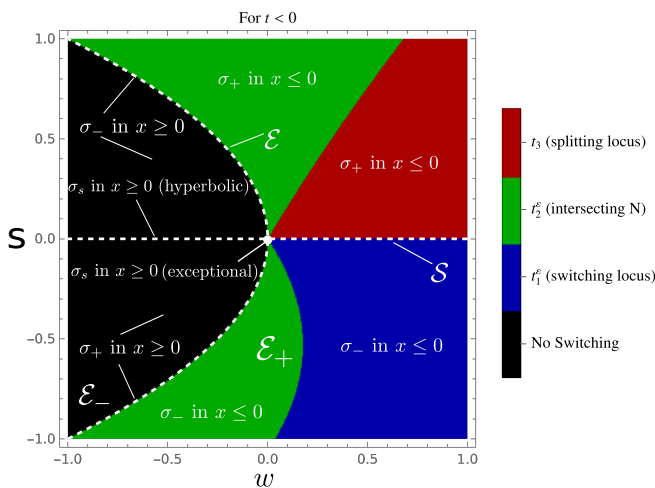


Fig. 5. Minimum time $t^* = \max(t_1^\varepsilon, t_2^\varepsilon, t_3)$ to reach $(0, w, s) \in N$ from a neighbourhood U of 0 for the model (5) with $b = b_1 = 1, c = 0$. The exceptional locus is $\mathcal{E} : y = -z^2$ and the singular locus is $\mathcal{S} : n \cdot [Y, X](q) = 0 : z = 0$.

2.3 Application to the McKeithan network

The collinearity locus. Another codimension two case occurs at the collinearity locus $\mathcal{C} = \{q \in N, X \text{ and } Y \text{ are collinear}\}$. This corresponds to singular points of the $2d$ -vector X and it occurs in the McKeithan network.

$\mathcal{C} \cap N$ leads to isolated singular points and in the generic case such a point is not a singular trajectory. We derive a semi-normal form at such point identified to 0 using the following normalization

- $X(0)$ and $Y(0)$ are collinear,
- X at 0 is not tangent to the curve $\mathcal{E} \cap N$,
- There is no singular trajectory arriving at 0,
- The collinearity locus $\mathcal{C} \cap N$ is transverse to $\mathcal{E} \cap N$ at 0 and it not tangent to X at 0.

Thus we obtain a model of the form $\dot{q} = Aq + ub$ and the local synthesis can be easily described with the method described above.

The stratification of the terminal manifold N is given in Fig. 6 and describes the codimension 2 situations of this network.

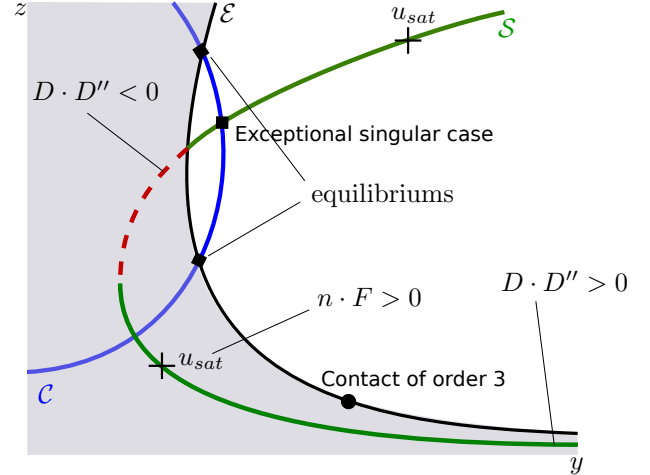


Fig. 6. Description of the codimension 2 cases analyzed in our section for the McKeithan network.

3. CONCLUSION

We presented a method to determine efficiently the local time minimal synthesis for optimal control problems and complete the work [Launay et al, 1997] using geometric analysis and formal computation in the exceptional situation of codimension 2.

This is applied to the control of the McKeithan network where complex situations appear. In the continuity of the study of this reversible network, we can extend the proposed techniques to treat an important problem related to the existence of equilibria corresponding to codimension 3 situations.

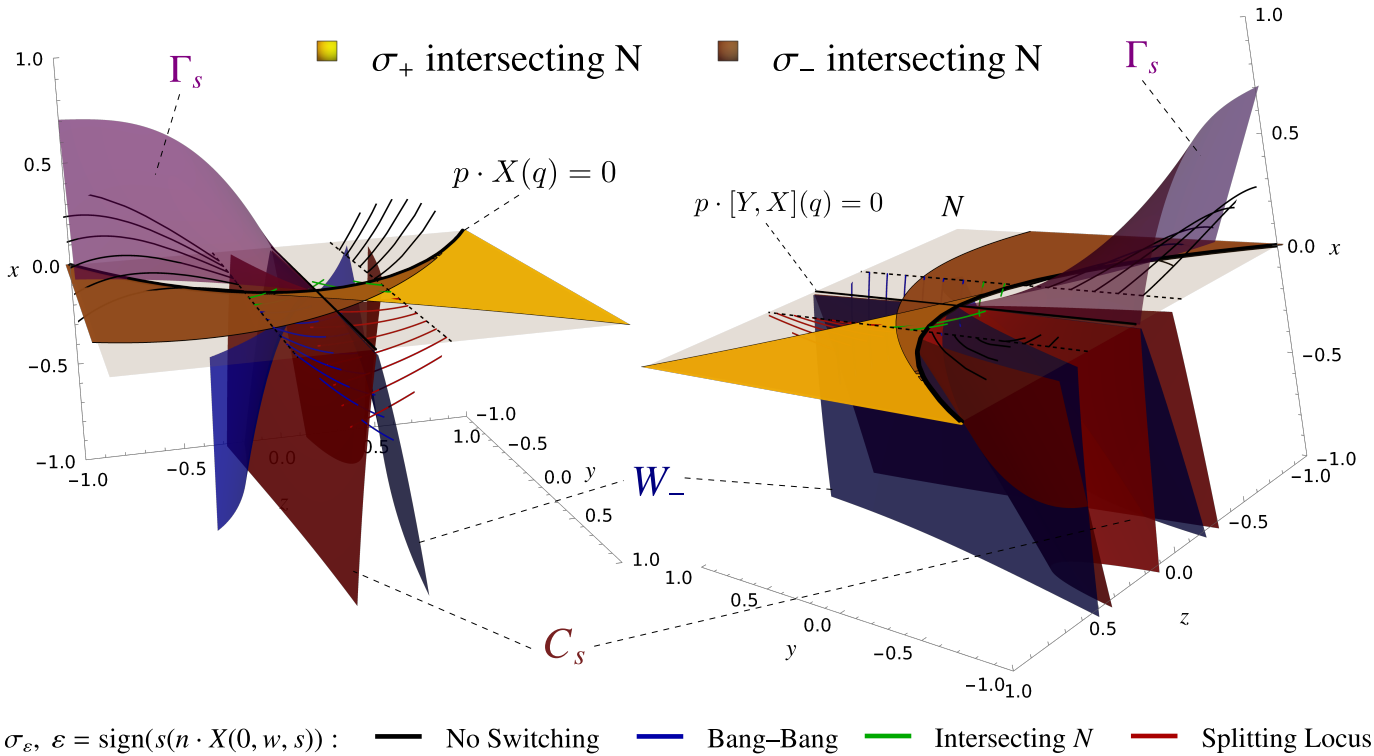


Fig. 4. Strata of the surface S separating the regions of U where the control is ± 1 for the model (5) with $b = b_1 = 1$, $c = 0$. We also represent the regions where σ_{\pm} intersect N for $t < 0$ and several trajectories which generate a switching locus and a splitting locus.

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