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# Connection between singular arcs in optimal control using bridges.

## Physical occurrence and Mathematical model

T. Bakir and B. Bonnard and J. Rouot

**Abstract**— In the time minimal control problem, singular arcs are omnipresent to determine the optimal solutions and leads to the well known turnpike phenomenon [1]. Very recently, this connection between singular arcs using a bang arc was shown to be relevant to saturate a single spin in Magnetic Resonance Imaging. Based on this example we propose a mathematical model to analyze such connection, which is called a bridge. This is applied to compute bridges in the optimization of chemical reaction networks using temperature control.

**Keywords:** Pontryagin maximum principle · Singularity theory · Geometric control

### I. INTRODUCTION

In this article we consider a real analytic *single input* control system in  $\mathbb{R}^{n-1}$  of the form:  $\frac{dc}{dt} = f(c, T) \in \mathbb{R}^{n-1}$ ,  $T \in \mathbb{R}$  which is extended using the *Goh transformation*  $u = \frac{dT}{dt}$  onto the control affine system

$$\frac{dx}{dt} = F(x) + u G(x), \quad x = (c, T) \in \mathbb{R}^n$$

and the set  $\mathcal{U}$  of admissible controls is the set of bounded measurable mappings defined on  $[0, t_f(u)]$ , and valued into  $[-1, 1]$  (such notations being motivated by the control of chemical reaction networks where  $c$  is the vector representing the concentrations of the chemical species and  $T$  is the temperature).

We consider the time-minimal control problem where  $x(0) = x_0$  is fixed and  $x(t_f) \in N$  where  $N$  is the (analytic) terminal manifold. According to the Maximum Principle [15] an optimal solution has to be found among the *extremal triplets*  $(x(\cdot), p(\cdot), u(\cdot))$ ,  $p \in \mathbb{R}^n \setminus 0$  solutions for a.e.  $t \in [0, t_f]$  of the pseudo-Hamiltonian system:

$$\dot{x}(t) = \frac{\partial H}{\partial p}(x(t), p(t), u(t)), \quad \dot{p}(t) = -\frac{\partial H}{\partial x}(x(t), p(t), u(t)), \quad (1)$$

$$H(x(t), p(t), u(t)) = M(x(t), p(t)) \quad (2)$$

where  $H(x, p, u) = p \cdot (F(x) + u G(x))$  is the *pseudo Hamiltonian*,  $\cdot$  stands for the scalar product and  $M(x, p) = \max_{|u| \leq 1} H(x, p, u)$  is the *maximized Hamiltonian*. Moreover  $M(x(t), p(t))$  is a non-negative constant along an extremal solution and one has  $p(t_f) \perp T_{x(t_f)}N$  (*transversality equation*).

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An extremal triplet is called

**Regular:** if  $u(t) = \text{sign } p(t) \cdot G(x(t))$  a.e. on  $[0, t_f]$ .

**Singular:** if  $u(t)$  is defined by the implicit relation

$$p(t) \cdot G(x(t)) = 0 \text{ a.e. on } [0, t_f]. \quad (3)$$

Note that a general extremal is a concatenation of such subcases.

In the second case, the singular control  $u_s(t)$  can be obtained differentiating twice the equation (3) as follows. Introducing the Lie bracket of two vector fields  $Z_1, Z_2$ :  $[Z_1, Z_2] = \frac{\partial Z_1}{\partial x}(x)Z_2(x) - \frac{\partial Z_2}{\partial x}(x)Z_1(x)$  one gets:

$$p(t) \cdot G(x(t)) = p(t) \cdot [G, F](x(t)) = 0 \quad (4)$$

$$p(t) \cdot ([G, F], F] + u(t) [[G, F], G])(x(t)) = 0 \quad (5)$$

From (5) if  $p(t) \cdot [[G, F], G](x(t))$  is non zero, the singular control  $u_s(t)$  can be defined as

$$u_s(t) = -\frac{p(t) \cdot [[G, F], F](x(t))}{p(t) \cdot [[G, F], G](x(t))}. \quad (6)$$

Moreover from the *high order Maximum Principle* [11], the so-called *Legendre-Clebsch condition*:

$$\frac{\partial}{\partial u} \frac{d^2}{dt^2} \frac{\partial H}{\partial u} = p(t) \cdot [[G, F], G](x(t)) \geq 0$$

is a necessary time optimality condition.

Connection between singular arcs and regular arcs are authorized to compute the optimal solutions and such connection occur when meeting the *switching surface*:  $\Sigma : p \cdot G(x) = 0$ . Such a phenomenon was analyzed in the generic case in the seminal article [12] and it can be used in many case to compute the so-called turnpike optimal solution of the form  $\sigma_{\pm} \sigma_s \sigma_{\pm}$  where  $\sigma_{\pm}$  is a bang arc and  $\sigma_s$  is a singular arc (the arc  $\sigma_1 \sigma_2$  represents an arc  $\sigma_1$  followed by  $\sigma_2$ ). The objective of this article is to analyze the connection between singular arcs using a *bridge* that is a bang arc which is tangent to  $\Sigma$  at both extremities, which leads to optimal solutions of the form  $\sigma_{\pm} \sigma_s \sigma_{\pm} \sigma_s \sigma_{\pm} \dots$ . This phenomenon was obtained in many cases in the problem of multisaturation of spin particles see [2] or [14] for a single spin, that is to drive the magnetization vector from the North pole to the center of the Bloch ball, where the system is of the form:

$$\dot{x} = -\Gamma x - uy, \quad \dot{y} = -\gamma(y - 1) + ux, \quad |u| \leq 1 \quad (7)$$

with  $0 < \gamma \leq 2\Gamma$ ,  $\Gamma, \gamma$  being the relaxation parameters.

The main contribution of this article is to present this important physical example to derive a mathematical model in dimension two, which can be easily generalized in higher dimension to provide a geometric tool to compute bridges

in general. In particular it can be used to complete our programs of optimizing the yield of batch chemical reactors by controlling the temperature [5], [4].

The organization of this article is the following. In section II, we present a recap of the classification of extremals near the switching surface in the so-called *fold case* [12] which is the basis of the geometric construction of bridges. In section III, the saturation of the spin case is described in details based on [2]. This leads to construct in section IV a planar mathematical model. Occurrence of bridges for chemical networks are computed in the final section.

## II. CONCEPT AND RECAP ABOUT THE CLASSIFICATION OF EXTREMALS [12]

### A. Notations

We denote by  $\sigma_+$  (resp.  $\sigma_-$ ) a bang arc which constant control  $+1$  (resp.  $-1$ ) and  $\sigma_s$  is a singular arc. We note  $\sigma_1\sigma_2$  an arc  $\sigma_1$  followed by  $\sigma_2$ . The surface  $\Sigma : p \cdot G(x) = 0$  is called the *switching surface*. If  $z(\cdot) = (x(\cdot), p(\cdot))$  is an extremal curve on  $[0, t_f]$ , we note  $\Phi(t) = p(t) \cdot G(x(t))$  the *switching function* (which codes the switching times). Differentiating twice with respect to time one gets:

$$\dot{\Phi}(t) = p(t) \cdot [G, F](x(t)), \quad (8)$$

$$\ddot{\Phi}(t) = p(t) \cdot ([G, F], F](x(t)) + u(t) [[G, F], G](x(t)). \quad (9)$$

From this calculus we deduce:

**Ordinary switching time.**  $t \in [0, t_f]$  is called an *ordinary switching time* and  $z(t)$  an *ordinary switching point* if  $\Phi(t) = 0$  and  $\dot{\Phi}(t) \neq 0$ . From that we deduce:

**Lemma 1.** *In the ordinary case, near  $z(t)$  every extremal solution is of the form  $\sigma_+\sigma_-$  if  $\dot{\Phi}(t) < 0$  and  $\sigma_-\sigma_+$  if  $\dot{\Phi}(t) > 0$ .*

**The Fold case.** If  $\Phi_\varepsilon(t) = \dot{\Phi}_\varepsilon(t) = 0$  and  $\ddot{\Phi}_\varepsilon(t) = p(t) \cdot ([G, F], F](x(t)) + \varepsilon [[G, F], G](x(t)) \neq 0$ ,  $\varepsilon = \pm 1$ , the point  $z(t) = (x(t), p(t))$  is called a *fold point*. If moreover  $p \cdot G(x) = p \cdot [G, F](x)$  is regular, we have three cases:

- Case 1. *parabolic case:*  $\ddot{\Phi}_+(t)\ddot{\Phi}_-(t) > 0$ .
- Case 2. *hyperbolic case:*  $\ddot{\Phi}_+(t) > 0$  and  $\ddot{\Phi}_-(t) < 0$ .
- Case 3. *elliptic case:*  $\ddot{\Phi}_+(t) < 0$  and  $\ddot{\Phi}_-(t) > 0$ .

Moreover denotes by  $u_s(t)$  the singular control defined by

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

one has

**Theorem 1.** *In a neighborhood of  $z(t)$  every extremal solution is of the form:*

- *Parabolic case:*  $\sigma_+\sigma_-\sigma_+$  or  $\sigma_-\sigma_+\sigma_-$
- *Hyperbolic case:*  $\sigma_\pm\sigma_s\sigma_\pm$
- *Elliptic case:* each extremal is bang-bang, i.e. of the form  $\sigma_+\sigma_-\sigma_+\sigma_-\dots$  but the number of switches is not uniformly bounded.

**The concept of bridge.** From the previous analysis, a *bridge* is a bang arc ( $\sigma_+^b$  or  $\sigma_-^b$ ) connecting two different hyperbolic points so that  $\sigma_\pm\sigma_s\sigma_\pm^b\sigma_s\sigma_\pm$  is an authorized extremal curve.

## III. THE OCCURRENCE OF (OPTIMAL) BRIDGES IN NMR [2]

We consider the problem of transferring the system from the North pole  $N = (0, 1)$  to the center  $O = (0, 0)$  of the Bloch ball so that the system takes the form

$$F = -\Gamma x \frac{\partial}{\partial x} + \gamma(1 - y) \frac{\partial}{\partial y}, \quad G = -y \frac{\partial}{\partial x} + x \frac{\partial}{\partial y}.$$

where  $\Gamma, \gamma$  are the relaxation parameters and  $0 < \gamma \leq 2\Gamma$ . Note that  $F$  is affine with a single stable node equilibrium at the North pole and integral curves of  $G$  are circles.

To make the analysis denoting  $\delta = \gamma - \Gamma$ , we need the following Lie brackets

$$[G, F] = (-\gamma + \delta y) \frac{\partial}{\partial x} + \delta x \frac{\partial}{\partial y},$$

$$[[G, F], F] = (\gamma(\gamma - 2\Gamma) - \delta^2 y) \frac{\partial}{\partial x} + \delta^2 x \frac{\partial}{\partial y},$$

$$[[G, F], G] = 2\delta x \frac{\partial}{\partial x} + (\gamma - \delta y) \frac{\partial}{\partial y}.$$

**Singular arcs.** They are located on the set  $S : \det(G, [G, F]) = 0$  which is given by  $x(\gamma - 2\delta y) = 0$ . Hence, they are two lines: the  $y$ -axis of symmetry and the horizontal line  $L : y_0 = \gamma/(2\delta)$ . These lines intersect the Bloch ball  $x^2 + y^2 < 1$  whenever  $2\Gamma > 3\gamma$  and moreover with  $y_0 < 0$ .

Along the vertical line, the singular control is zero and along  $L$  it is given by:  $D'(x) + u_s D(x) = 0$  where  $D = \det(G, [[G, F], G])$  and  $D' = \det(G, [[G, F], F])$ . Computing we have  $u_s = \gamma(2\Gamma - \gamma)/(2\delta)x$  and  $u_s \rightarrow \infty$  when  $x \rightarrow 0$ .

The strict Legendre-Clebsch condition from [11] is used to distinguish between fast and slow displacement direction. Introducing  $D'' = \det(G, F)$  we have: fast if  $DD'' > 0$  and slow if  $DD'' < 0$ .

Computing we have:

- The horizontal line is fast
- The vertical line is fast if  $1 > y > y_0 = \gamma/(2\delta)$  and slow if  $y_0 = \gamma/(2\delta) > y > -1$ .

We represent in Fig.1 the optimal policy to drive the North pole to the center  $O$  computed for parameters such that  $0 < 3\gamma < 2\Gamma$ . By symmetry we represent the policy in the domain  $x < 0$ . Note that the bridge occurs at  $S_2$  before the *saturating point*  $S_3$  where  $|u_s| = 1$ . The optimal policy is  $\sigma_+\sigma_s^h\sigma_+^b\sigma_s^v$  where  $\sigma_s^h, \sigma_s^v$  are respectively the horizontal and vertical singular arc,  $\sigma_+^b$  is the bridge. This policy can be compared to the standard inversion sequence  $\sigma_+\sigma_s^v$  used in practice.

From the previous analysis one use the following in terms of Lie brackets at  $(0, y_0)$  which is the intersection of the singular lines:

$$p \cdot [[G, F], G](0, y_0) = 0.$$

Moreover  $p \cdot [[G, F], G](0, y_0) > 0$  for  $y > y_0$  and  $< 0$  if  $y < y_0$  and  $p$  can be seen on the picture thanks to the relation  $p \cdot G(x) = 0$ . Conditions on the parameters to have a bridge can be obtained computing Lie brackets up to order 4 at  $(0, y_0)$ .

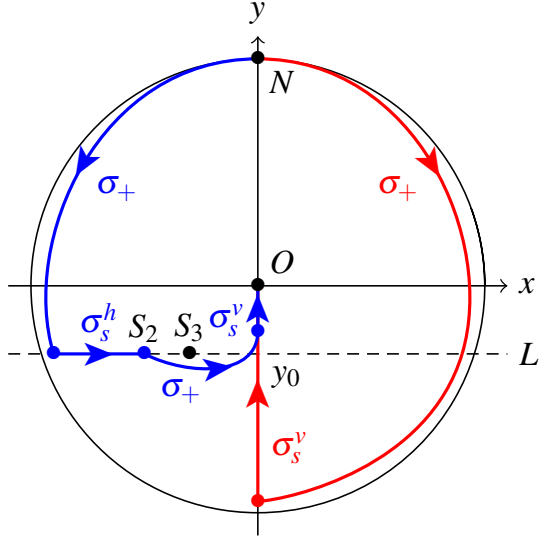


Fig. 1. (left) Time optimal policy with a bridge compared with (right) inversion sequence.

#### IV. CONSTRUCTION OF A PLANAR (SYMMETRIC) MODEL

From the previous example we shall construct a *local model* (near  $(0, y_0)$  in the previous example) which exhibits the previous behaviors.

##### A. Birth of the model.

We start with the following planar model:

$$\begin{cases} \dot{x} = u \\ \dot{y} = 1 - \varepsilon y^2 \end{cases}$$
 where the singular arc  $\sigma_s$  is identified to  $t \mapsto (0, t)$  and corresponds to  $u_s(t) = 0$ . Such a line is fast if  $\varepsilon > 0$  and slow if  $\varepsilon < 0$ . Moreover we have  $[G, F] = 2xy \frac{\partial}{\partial y}$  and  $[[G, F], G] = x \frac{\partial}{\partial y}$ . Hence singular trajectories are the two lines:  $x = 0$  and  $y = 0$ . By construction the vertical line can be followed by  $u = 0$  and the horizontal line can be followed by " $u = \infty$ " so it cannot be tracked in practice. To construct the model one must bend this line and we get the following.

##### B. The model

We consider the system

$$\dot{\mathbf{x}} = F(\mathbf{x}) + u G(\mathbf{x}), \quad t_f \leftarrow \min_{|u| \leq 1}, \quad \mathbf{x} = (x, y) \quad (10)$$

where  $F = (1 - x^2 y) \frac{\partial}{\partial x}$  and  $G = -(y - 1) \frac{\partial}{\partial x} + x \frac{\partial}{\partial y}$ . Note that integrating  $G$  led to circles centered at  $x = 0, y = 1$ .

**Computations.** We have

- $[G, F](x, y) = (-1 + x^2 y) \frac{\partial}{\partial x} + (2xy(1 - y) + x^3) \frac{\partial}{\partial y}$ ,
- $[[G, F], G](x, y) = 2x(x^2 - 2(y - 1)y) \frac{\partial}{\partial x} + (x^2(5 - 8y) + 2y^3 - 4y^2 + 2y + 1) \frac{\partial}{\partial y}$ ,
- $[[G, F], F](x, y) = (x^2 - x^4 y) \frac{\partial}{\partial x} + x(x^4 + 4x^2 y^2 - 6y + 2) \frac{\partial}{\partial y}$ ,
- $\det(G, [G, F])(x, y) = x(x^2(1 - 2y) + 2y^3 - 4y^2 + 2y + 1)$ ,
- $D(x, y) = \det(G, [[G, F], G]) = -2x^4 + x^2(12y^2 - 17y + 5) - 2y^4 + 6y^3 - 6y^2 + y + 1$ ,

- $D'(x, y) = \det(G, [[G, F], F]) = x(x^4 + x^2(-4y^3 + 4y^2 - 1) + 6y^2 - 8y + 2)$ ,
- Collinearity set:  $D''(x, y) = 0$  with  $D''(x, y) = \det(G, F) = (y - 1)(x^2 y - 1)$ .

**Singular trajectories.** The singular set is defined by  $\Sigma_s = \{q, \det(G, [G, F])(q) = 0\}$  and we have

**Lemma 2.** The singular trajectories corresponds to the union of the vertical line  $(Oy)$  and the algebraic curve defined by  $l(x, y) := x^2(1 - 2y) + 2y^3 - 4y^2 + 2y + 1 = 0$ .

**Remark 1.** The equation  $l(x, y) = 0$  is equivalent to  $x = \pm \sqrt{\frac{2y^3 - 4y^2 + 2y + 1}{2y - 1}}$  and we denote by  $\mathcal{L}$  the component of the curve where  $y \leq y_0$  and by  $\mathcal{L}'$  the component of the curve where  $y \geq y_0$  (see Fig.2).

Moreover  $\Sigma_s \cap (Oy) = \{(0, y_0)\}$  where  $y_0 \simeq -0.297157$  is the unique real root of  $l(0, y) = 0$ .

**Bridge bang arc.** Consider the problem of minimizing the time to reach the origin starting from the point  $(x(0), y(0)) = (-1, -1)$  and under the dynamics defined by (10). A time minimal solution is of the form  $\sigma_- \sigma_s \sigma_+^b \sigma_s$  where  $\sigma_-$  is a bang arc associated to  $u = -1$ ,  $\sigma_s$  is a singular arc and  $\sigma_+^b$  is a bridge that is a bang arc connecting two points of the singular line. We represent in Fig.4-5 the extremal associated to this solution.

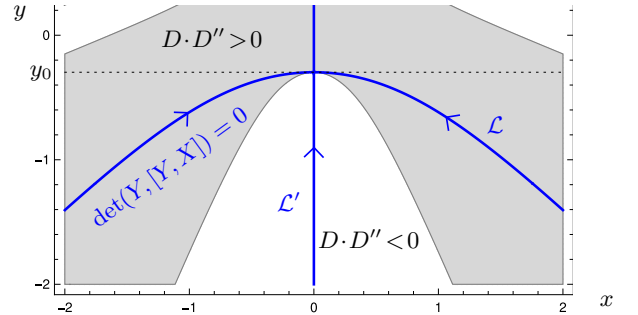


Fig. 2.  $(Oy)$  and  $\mathcal{L}$  are two singular trajectories for the system (10) represented by two continuous lines. The dash-dotted curve corresponds to the collinearity set. The filled regions are the points where  $D \cdot D'' > 0$ .

From the following computations

- along  $(Oy)$ ,  $D \cdot D'' = (y - 1)^2 (2y^3 - 4y^2 + 2y + 1)$ ,
- along  $\mathcal{L}$ ,  $D \cdot D'' = 2(79y_0^2 - 120y_0 + 74)(y_0 - y)/(1 - 2y_0)^4 + o(y - y_0)$ ,

we have

**Proposition 1.** The vertical singular line  $(Oy)$  is hyperbolic for  $y > y_0$ , elliptic for  $y < y_0$ . The singular trajectory  $\mathcal{L}$  is hyperbolic.

The singular control along  $(Oy)$  is zero and the expression of the singular control along  $\mathcal{L} \cap \{x \leq 0\}$  is

$$u_s = -\frac{D'}{D} = \frac{-8y^7 + 30y^6 - 44y^5 + 38y^4 - 27y^3 + 15y^2 - 6y + 2}{\sqrt{(2y - 1)(2y^3 - 4y^2 + 2y + 1)}(8y^3 - 15y^2 + 9y - 3)}$$

and  $u_s$  is represented in Fig. 3.

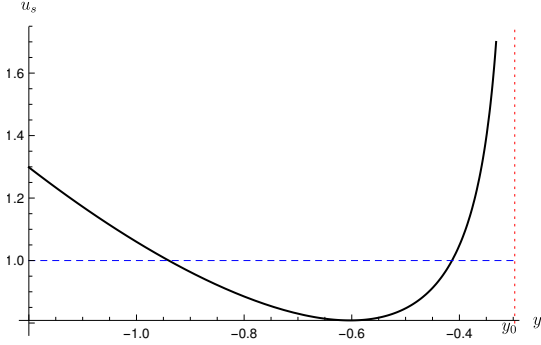


Fig. 3. Singular control  $u_s$  for  $x < 0$ . There exists two saturating points.

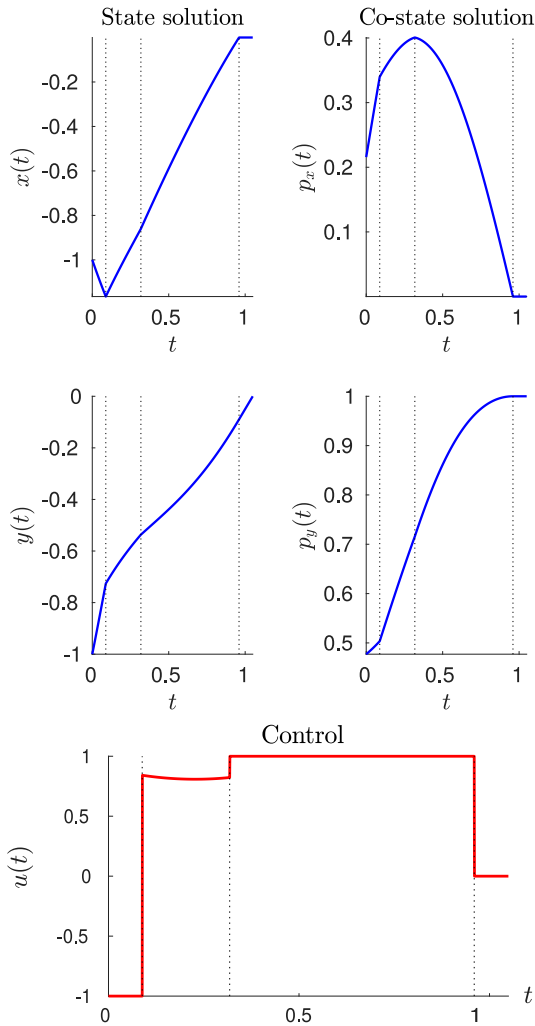


Fig. 4. Time evolution of an extremal for the problem (10) of reaching the origin in minimal time starting from  $(x(0), y(0)) = (-1, -1)$ .

**Remark 2.** Adding a parameter  $\lambda$  in the model (10) by replacing the vector field  $G$  by  $G \leftarrow -(y - \lambda) \frac{\partial}{\partial x} + x \frac{\partial}{\partial y}$  affects the position of  $y_0$  (see Fig.6): as  $\lambda \rightarrow +\infty$ ,  $y_0 \rightarrow 0$ .

By rescaling one can make  $y_0 \rightarrow 0$  and this leads to a complicated synthesis near 0.

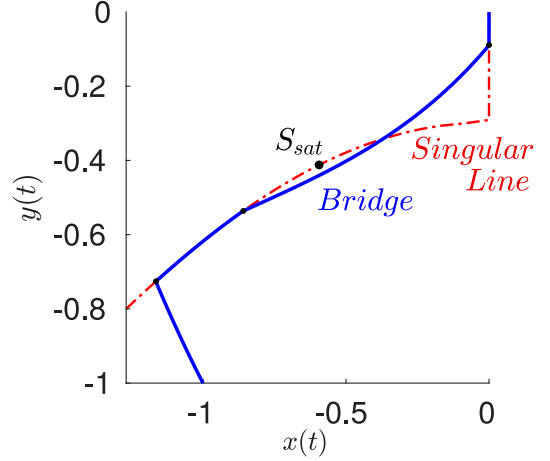


Fig. 5. Trajectory associated to the extremal of Fig.4.  $\sigma_+^b$  is a bridge connecting two switching points of the singular set and the singular control saturates at the point  $S_{sat}$ .

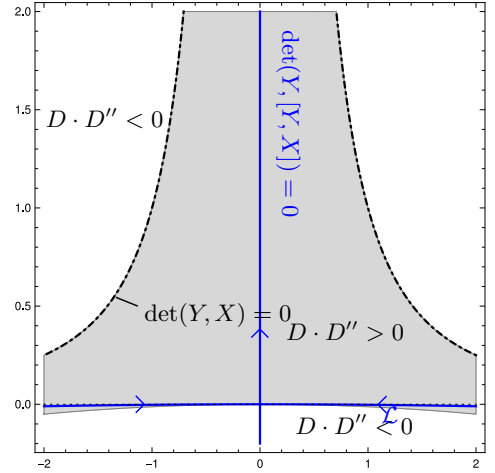


Fig. 6.  $(Oy)$  and  $\mathcal{L}$  corresponding singular trajectories for the system (10) where  $G$  is replaced by  $G = -(y - \lambda) \frac{\partial}{\partial x} + x \frac{\partial}{\partial y}$  and  $\lambda = 200$ . The dash-dotted curve corresponds to the collinearity set. The filled regions are the points where  $D \cdot D'' > 0$ .

**Remark 3.** Interaction between two singular lines is coded by the singularities of the flow:  $\dot{x} = F(x) - \frac{D'(x)}{D(x)} G(x)$  since  $D' + u_s D = 0$ . It can be analyzed using time reparameterization to lead to  $\dot{x} = D(x)F(x) - D'(x)G(x)$ . This geometric remark is crucial for the extension to the non planar case that we present next.

## V. EXTENSION TO THE $n$ -DIMENSIONAL CASE AND AN APPLICATION TO CHEMICAL NETWORKS

### A. Extension

Due to the space restriction we shall consider the situation  $n = 3$ , which already contains all the technical difficulties. In this case, we introduce the following determinants:

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

and from (4)-(5)-(6) the singular control is given by

$$u_s(x) = -\frac{D'(x)}{D(x)}.$$

We have three types of singular trajectories coming from the fold case classification:

- *hyperbolic*:  $D D'' > 0$
- *elliptic*:  $D D'' < 0$

and the so-called *exceptional case* corresponds to singular trajectories such that  $H = p \cdot F(x) = 0$ . Eliminating  $p$  leads to

- *exceptional*:  $D'' = 0$ .

Note that in this case the adjoint vector is either  $p$  or  $-p$ .

Moreover using [3] the small time optimality status is: time minimizing in the hyperbolic and exceptional case, time maximizing in the elliptic case.

Again, since the singular trajectories are solutions of:  $\dot{x} = F(x) - \frac{D'(x)}{D(x)}G(x)$  connections between singular arcs are related to the behaviors of the solution of the reparameterized equation:

$$\dot{x} = D(x)F(x) - D'(x)G(x)$$

and in particular near the *non isolated equilibria* contained in  $D = D' = 0$ .

This is the main issue for  $n \geq 3$  to analyze connections between singular arcs using a bridge in relation with the occurrence of  $p(t) \cdot [[G, F], G](x(t)) = 0$ .

### B. Application to chemical networks

We shall outline the discussion of the occurrence of bridges for chemical networks, extending results from [5], [4]. The problem of maximizing the yield of one species  $[X]$  is converted into a minimizing the time to produce a fixed  $[X] = d$  ( $[X]$  denoting the concentration of the species  $X$ ).

One consider two reactions schemes:

**Case 1:**  $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ : sequence of two irreversible reactions  $k_i = A_i \exp(-E_i/(RT))$ ,  $i = 1, 2$ ,  $A_i, E_i$  are parameters,  $R$  is the gas constant and  $T$  is the temperature.

We introduce  $v = k_1$ ,  $x = \log[A]$ ,  $y = [B]$ ,  $\alpha = E_2/E_1$ ,  $\beta = A_2/A_1^\alpha$  so that the dynamics takes the form:  $F = -vx \frac{\partial}{\partial x} + (vx - \beta v^\alpha y) \frac{\partial}{\partial y}$ ,  $G = \frac{\partial}{\partial v}$  and the terminal manifold is  $N = \{[B] = y = d\}$ . Computing one has

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

One wants to detect the existence of bridges near the terminal manifold. In the discussion we introduce the following stratification of  $N$ .

- $\mathcal{E}$ : *exceptional set*:  $n \cdot F = 0$  with  $n = (0, 1, 0)$  normal to  $N$  and we get  $\mathcal{E}: vx - \beta y v^\alpha = 0$ ,
- $\mathcal{S}$ : *singular arcs* so that  $n \cdot G = n \cdot [G, F] = 0$ , that is  $-x + \alpha \beta y v^{\alpha-1} = 0$ .

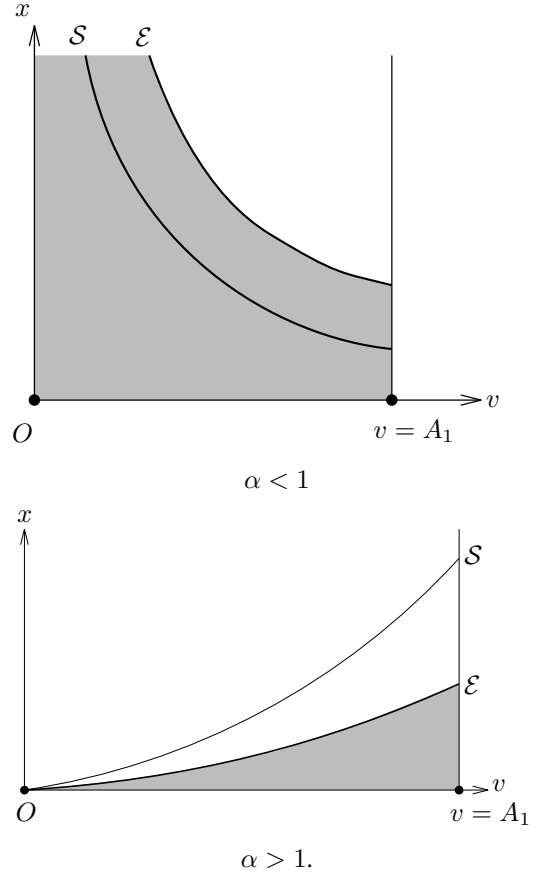


Fig. 7. Stratification of the manifold  $N$ .

We represent  $\mathcal{E}$  and  $\mathcal{S}$  on Fig.7 in the two cases  $\alpha > 1$  and  $\alpha < 1$ .

Note that  $\mathcal{E}$  forms the boundary of the terminal manifold which can be reached from  $y(0) < d$ . In case  $\alpha > 1$ , there exists no admissible singular arcs and the optimal policy is  $u = +1$ . In the case  $\alpha < 1$ , there exists hyperbolic singular arcs.

**Case 2:** Consider now the following network where the first reaction is reversible:  $A \xrightleftharpoons[k_3]{k_1} B \xrightarrow{k_2} C$  where  $k_i = A_i \exp(-E_i/(RT))$ ,  $i = 1, 2, 3$ . Denote  $v = k_1$ ,  $\alpha = E_2/E_1$ ,  $\alpha' = E_3/E_1$ ,  $\beta = A_2/A_1^\alpha$ ,  $\beta' = A_3/A_1^{\alpha'}$ ,  $x = [A]$ ,  $[y] = [B]$  so that the dynamics is defined by  $F = (-vx + \beta' v^{\alpha'} y) \frac{\partial}{\partial x} + (vx - \beta' v^{\alpha'} y - \beta v^\alpha y) \frac{\partial}{\partial y}$  and  $G = \frac{\partial}{\partial v}$ . One has

- $[G, F] = (x - \alpha' \beta' v^{\alpha'-1} y) \frac{\partial}{\partial x} + (-x + \alpha' \beta' v^{\alpha'-1} y + \alpha \beta v^{\alpha-1} y) \frac{\partial}{\partial y}$ ,
- $[[G, F], G] = (-\alpha'(\alpha'-1)\beta' v^{\alpha'-2} y) \frac{\partial}{\partial x} + (\alpha'(\alpha'-1)\beta' v^{\alpha'-2} y + \alpha(\alpha-1)\beta v^{\alpha-2} y) \frac{\partial}{\partial y}$ ,
- $D = \det(G, [G, F], [[G, F], G]) = \alpha(\alpha-1)\beta x y v^{\alpha-2} + \alpha' \beta' \alpha \beta (\alpha' - \alpha) v^{\alpha+\alpha'-3} y^2$
- $D' = \det(G, [G, F], [[G, F], F]) = y^2 (\alpha \beta^2 \beta' (\alpha - \alpha') v^{2\alpha+\alpha'-2} - \alpha' \beta \beta'^2 (\alpha' - \alpha) v^{\alpha+2\alpha'-2} + \beta (\alpha \alpha' \beta' - \alpha \beta') v^{\alpha+\alpha'-1}) + \beta x y (2\alpha' \beta' - 2\alpha \beta') v^{\alpha+\alpha'-1} + (\alpha - 1) \beta x^2 v^\alpha$

- $D'' = \det(G, [G, F], F) = -\beta v^\alpha xy + (\alpha' - \alpha)\beta\beta'v^{\alpha'+\alpha-1}y^2$ .

Computing  $\mathcal{E}$  and  $\mathcal{S}$  with  $y = d$  leads to

- *exceptional case*:  $\mathcal{E} : n \cdot F = vx - v^{\alpha'}d(\beta v^{\alpha-\alpha'} + \beta') = 0$ .
- *singular case*:  $\mathcal{S} : n \cdot [G, F] = dv^{\alpha'-1}(\alpha\beta v^{\alpha-\alpha'} + \alpha'\beta') - x = 0$ .

From which we deduce that  $\mathcal{E} \cap \mathcal{S}$  is defined by

$$x = d\beta'v^{\alpha'-1}\frac{\alpha - \alpha'}{\alpha - 1}$$

$$v^{\alpha-\alpha'} = -\frac{\beta'(\alpha' - 1)}{\beta(\alpha - 1)}.$$

We represent on Fig.8,  $\mathcal{E}$  and  $\mathcal{S}$  for specific values of the parameters such that

- $\mathcal{E} \cap \mathcal{S} \neq \emptyset$
- A bridge occurs and corresponds to a vertical tangent to  $\mathcal{S}$  at the point  $(x, v)$  where  $n \cdot [[G, F], G](x, v) = 0$ .

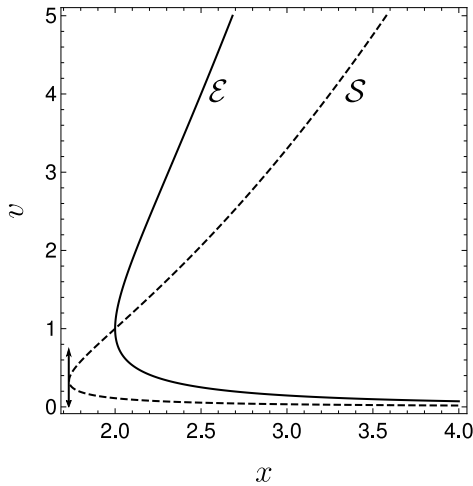


Fig. 8. Stratification of  $N : y = d$  for  $d = 1, \alpha = 1.5, \beta = \beta' = 1, \alpha' = 0.5$ .  $\mathcal{S} = \{n \cdot G = n \cdot [G, F] = 0\}$ ,  $\mathcal{E} = \{n \cdot F = 0\}$ .

## VI. CONCLUSION

In view of applications to optimize the yield of chemical batch reactors we have analyzed the so-called bridge phenomenon in optimal control that is a connection between two singular arcs using a bang arc. Based on the occurrence of this phenomenon in Magnetic Resonance Imaging we have constructed a planar mathematical model to analyze this phenomenon. This is extended in dimension 3 to describe cases where bridges can occur for chemical networks, in relation with reversibility.

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