



**HAL**  
open science

## Optimization of chemical batch reactors using temperature control

Jérémy Rouot, Bernard Bonnard

► **To cite this version:**

Jérémy Rouot, Bernard Bonnard. Optimization of chemical batch reactors using temperature control. 58 th Conference on Decision and Control, Dec 2019, Nice, France. hal-02483377

**HAL Id: hal-02483377**

**<https://inria.hal.science/hal-02483377>**

Submitted on 18 Feb 2020

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

# Optimization of chemical batch reactors using temperature control

Jérémy Rouot

ISEN, Brest, France

58<sup>th</sup> Conference on Decision and Control  
Nice, France  
December 11<sup>th</sup>-13<sup>th</sup> 2019

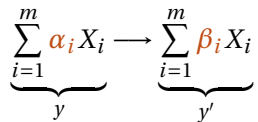
*joint work with B. Bonnard (INRIA & UBFC)*

# Chemical Networks with mass action kinetics

## Graph Model :

Species  $\{X_1, \dots, X_m\}$ .

Notations :  $\mathcal{R}$  is the set of reactions of the form :



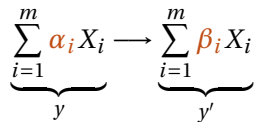
$\alpha_i, \beta_i$  are the stoichiometric coefficients.

# Chemical Networks with mass action kinetics

## Graph Model :

Species  $\{X_1, \dots, X_m\}$ .

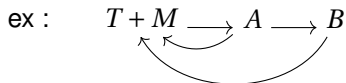
Notations :  $\mathcal{R}$  is the set of reactions of the form :



$\alpha_i, \beta_i$  are the stoichiometric coefficients.

## Feinberg-Horn-Jackson graph

- Vertices :  $\mathbf{y} = (\alpha_1, \dots, \alpha_m)^\top$ ,  $\mathbf{y}' = (\beta_1, \dots, \beta_m)^\top$
- Orientation :  $\mathbf{y} \rightarrow \mathbf{y}'$



**Rate dynamics  $\mathbf{y} \rightarrow \mathbf{y}'$  (Mass kinetics)**

$$K(\mathbf{y} \rightarrow \mathbf{y}') = k(T) c^{\mathbf{y}}$$

- $k(T) = A \exp(-\frac{E}{RT})$  : Arrhenius law  
 $E, A$  parameters,  $T$  temperature and  $R$  is the gas constant

## Rate dynamics $\mathbf{y} \rightarrow \mathbf{y}'$ (Mass kinetics)

$$K(\mathbf{y} \rightarrow \mathbf{y}') = k(T) c^{\mathbf{y}}$$

- $k(T) = A \exp(-\frac{E}{RT})$  : Arrhenius law  
 $E, A$  parameters,  $T$  temperature and  $R$  is the gas constant
- $\mathbf{c} = (c_1, \dots, c_m)^\top$   
 $c_i$  : concentrations of the species  $X_i$  with

$$c^{\mathbf{y}} = c_1^{\alpha_1} \dots c_m^{\alpha_m}$$

$\Rightarrow K(\mathbf{y} \rightarrow \mathbf{y}')$  depends only on  $\mathbf{y}$ .

## Dynamics for the network

$$\dot{\mathbf{c}}(\mathbf{t}) = F(\mathbf{c}(\mathbf{t}), T) = \sum_{\mathbf{y} \rightarrow \mathbf{y}' \in \mathcal{R}} K(\mathbf{y} \rightarrow \mathbf{y}') (\mathbf{y}' - \mathbf{y})$$

The dynamics is defined by the graph.

# Dynamics for the network

$$\dot{\mathbf{c}}(\mathbf{t}) = F(\mathbf{c}(\mathbf{t}), T) = \sum_{\mathbf{y} \rightarrow \mathbf{y}' \in \mathcal{R}} K(\mathbf{y} \rightarrow \mathbf{y}') (\mathbf{y}' - \mathbf{y})$$

The dynamics is defined by the graph.

- **Stoichiometric subspace**

$$S = \text{span} \{ \mathbf{y} - \mathbf{y}', \mathbf{y} \rightarrow \mathbf{y}' \in \mathcal{R} \}$$

- **Positive class** (strict if  $> 0$ )

$$(\mathbf{c}(\mathbf{0}) + S) \cap \mathbb{R}_{\geq 0}^m$$

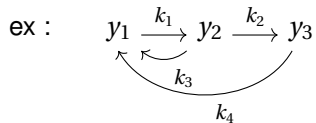
## Lemma

The class  $(\mathbf{c}(\mathbf{0}) + S) \cap \mathbb{R}_{> 0}^m$  is **invariant** for the dynamics.



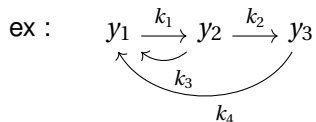
# Notations

- Labeling the vertices :  $y_1, y_2, \dots, y_n$



# Notations

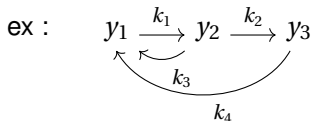
- Labeling the vertices :  $y_1, y_2, \dots, y_n$



- Complex matrix** :  $Y = (y_1, \dots, y_n)$  ( $n$  : number of vertices).

# Notations

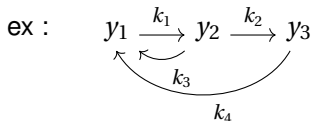
- Labeling the vertices :  $y_1, y_2, \dots, y_n$



- Complex matrix** :  $Y = (y_1, \dots, y_n)$  ( $n$  : number of vertices).
- Incidence connectivity matrix** :  $A = (a_{ij})_{ij}$   
with for instance  $a_{21} = k_1$  indicating a reaction with constant  $k_1$  from the first node of the graph to the second :  $y_1 \xrightarrow{k_1} y_2$

# Notations

- Labeling the vertices :  $y_1, y_2, \dots, y_n$



- Complex matrix** :  $Y = (y_1, \dots, y_n)$  ( $n$  : number of vertices).
- Incidence connectivity matrix** :  $A = (a_{ij})_{ij}$   
with for instance  $a_{21} = k_1$  indicating a reaction with constant  $k_1$  from the first node of the graph to the second :  $y_1 \xrightarrow{k_1} y_2$
- Laplacian matrix** :

$$\tilde{A} = A - \text{diag} \left( \sum_{i=1}^n a_{i1}, \dots, \sum_{i=1}^n a_{in} \right)$$

One has

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

where  $\mathbf{c}^Y = (c^{y_1}, \dots, c^{y_n})^\top$ .

# Zero deficiency theorem

## Definition (Deficiency)

*Feinberg and Horn-Jackson : articles in Archive Rational Mechanics*

**Graph concept** : deficiency :  $\delta = n - l - s$  where

- $n$  : number of vertices
- $l$  : number of connected components
- $s$  : dimension of the stoichiometric subspace

## Definition

The network is **weakly reversible** if  $\forall$  vertices  $(i, j)$  such that  $\exists$  oriented path joining  $i$  to  $j$ , there exists an oriented path joining  $j$  to  $i$ .

Assumption  $\delta = \mathbf{0}$  (Zero deficiency assumption)

## Theorem

- ① If the network is **not weakly reversible** then for arbitrary kinetics, the differential equation **cannot have a positive equilibrium nor a positive periodic trajectory**.
- ② If the network is **weakly reversible**, there exists within each strictly positive compatibility class precisely **one equilibrium**  $c^*$ , this equilibrium is locally asymptotically stable with (pseudo-Helmholtz) Lyapunov function  $V(c, c^*) = \sum_i [c_i(\ln(c_i) - \ln(c_i^*)) - 1] + c_i^*$ .  
Moreover there are no non trivial periodic orbits.





# Equilibrium for the McKeithan network

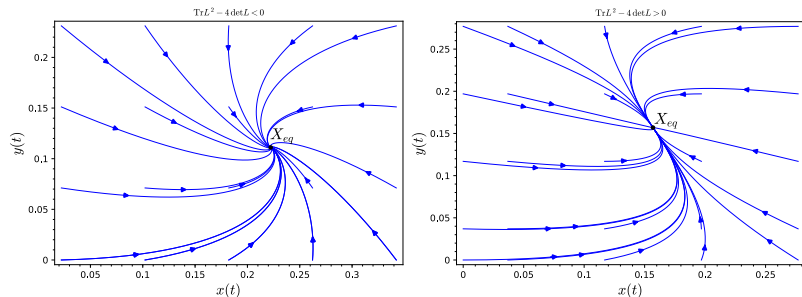


FIGURE – Phase portrait for the McKeithan model. (left) Focus ; (right) Node.

# Geometric Optimal Control

# Optimal Control Problem

$$\frac{d\mathbf{c}}{dt} = f(\mathbf{c}, T), \quad \frac{dT}{dt} = u, \quad u \in [u_-, u_+]$$

$u(\cdot)$  tracked the derivative of the temperature (related to the Goh Transformation).

Single input  $C^\omega$ -control system, affine in  $u$  :

$$\begin{cases} \dot{\mathbf{q}} = F(\mathbf{q}) + uG(\mathbf{q}), & |u| \leq 1, \\ \mathbf{q} = (\mathbf{c}, T) \in \mathbb{R}^n \end{cases}$$

## Formulation :

$$\max \mathbf{c}_1(t_f) \quad t_f : \text{(fixed) time batch duration}$$

## Formulation :

$$\max \mathbf{c}_1(t_f) \quad t_f : \text{(fixed) time batch duration}$$

Formulated as

$$\begin{cases} \min t_f \quad \text{(free)}, & |u| \leq 1 \\ \mathbf{c}_1(t_f) = d \text{ is a desired quantity} \end{cases}$$

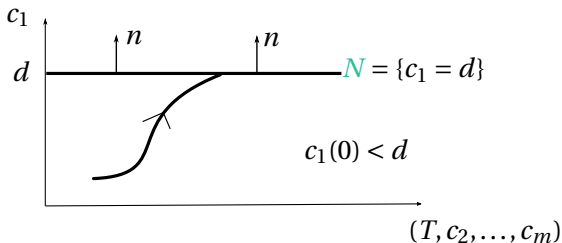
## Formulation :

$$\max c_1(t_f) \quad t_f : \text{(fixed) time batch duration}$$

Formulated as

$$\begin{cases} \min t_f \quad \text{(free)}, & |u| \leq 1 \\ c_1(t_f) = d \text{ is a desired quantity} \end{cases}$$

$N$  : terminal manifold of codimension 1.



# Necessary optimality conditions Pontryagin Maximum Principle (1956)

## Notations :

$$\begin{cases} \dot{\mathbf{q}} = F(\mathbf{q}) + uG(\mathbf{q}), & |u| \leq 1, \\ \min t_f, & \mathbf{q}(t_f) \in \mathbf{N} \end{cases}$$

- $H(\mathbf{q}, p, u) = p \cdot (F(\mathbf{q}) + uG(\mathbf{q}))$ ,  $p \in \mathbb{R}^n \setminus \{0\}$  : adjoint vector
- $H$  : pseudo-Hamiltonian and the maximized Hamiltonian is

$$M(\mathbf{q}, p) = \max_{|u| \leq 1} H(\mathbf{q}, p, u), \quad \mathbf{q}, p \text{ are fixed}$$

## Theorem

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

$$\dot{q}^*(\cdot) = \frac{\partial H}{\partial p}(q^*(t), p^*(t), u^*(t)), \quad \dot{p}^*(\cdot) = -\frac{\partial H}{\partial q}(q^*(t), p^*(t), u^*(t)) \quad (1)$$

the maximization condition is satisfied

$$H(q^*(t), p^*(t), u^*(t)) = M(q^*(t), p^*(t)). \quad (2)$$



## Theorem

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

$$\dot{q}^*(\cdot) = \frac{\partial H}{\partial p}(q^*(t), p^*(t), u^*(t)), \quad \dot{p}^*(\cdot) = -\frac{\partial H}{\partial q}(q^*(t), p^*(t), u^*(t)) \quad (1)$$

the maximization condition is satisfied

$$H(q^*(t), p^*(t), u^*(t)) = M(q^*(t), p^*(t)). \quad (2)$$

Moreover

- $t \mapsto M(q^*(t), p^*(t))$  is constant and  $\geq 0$ ,
- At the final time one has the transversality condition :

$$p^*(t_f) \perp T_{q^*(t_f)} \mathbf{N} \quad (3)$$

**Extremals** : solutions of (1)–(2).

**BC-extremal** : Extremals & transversality condition (3) satisfied.

### Maximization condition

- *regular* :  $p(t) \cdot G(\mathbf{q}(t)) \neq 0$

$$u(t) = \text{sign} (p(t) \cdot G(\mathbf{q}(t))) \text{ a.e.}$$

Finite number of switches : **Bang-Bang**

- *singular* :

$$p(t) \cdot G(\mathbf{q}(t)) = 0 \quad \forall t$$

# Computations of singular extremals and properties

**Notation :**  $X, Y$  : two vector fields on  $\mathbb{R}^n$

*Lie bracket :*

$$[X, Y](q) = \frac{\partial X}{\partial q}(q)Y(q) - \frac{\partial Y}{\partial q}(q)X(q)$$

$z = (q, p)$  and Hamiltonian lift of  $X$  :  $H_X(z) = p \cdot X(q)$

*Poisson bracket :*

$$\{H_X, H_Y\}(z) = p \cdot [X, Y](q)$$

# Computations of singular extremals and properties

**Notation :**  $X, Y$  : two vector fields on  $\mathbb{R}^n$

*Lie bracket :*

$$[X, Y](q) = \frac{\partial X}{\partial q}(q)Y(q) - \frac{\partial Y}{\partial q}(q)X(q)$$

$z = (q, p)$  and Hamiltonian lift of  $X$  :  $H_X(z) = p \cdot X(q)$

*Poisson bracket :*

$$\{H_X, H_Y\}(z) = p \cdot [X, Y](q)$$

**Computations**  $H_G(z) = p \cdot G(q) = 0$

Differentiating twice w.r.t. time gives the two equations

$$\frac{d}{dt} H_G(z) = dH_G \cdot \dot{z} = \{H_G, H_F + u H_G\} = \{\mathbf{H}_G, \mathbf{H}_F\} = \mathbf{0}$$

$$\{\{\mathbf{H}_G, \mathbf{H}_F\}, \mathbf{H}_F\}(z) + u \{\{\mathbf{H}_G, \mathbf{H}_F\}, \mathbf{H}_G\}(z) = \mathbf{0}$$

Then if  $\{\{H_G, H_F\}, H_G\}(z) \neq 0$  then we compute  $\hat{u}$  and plug it in  $H$  to obtain the *true Hamiltonian*.

## Generalized Legendre-Clebsch condition

$$\{\{H_G, H_F\}, H_G\}(z) \geq 0$$

⇒ necessary optimality condition (High Order Maximum Principle, Krener).

## Strict generalized Legendre-Clebsch condition

$$\{\{H_G, H_F\}, H_G\}(z) > 0$$

## Generalized Legendre-Clebsch condition

$$\{\{H_G, H_F\}, H_G\}(z) \geq 0$$

⇒ necessary optimality condition (High Order Maximum Principle, Krener).

## Strict generalized Legendre-Clebsch condition

$$\{\{H_G, H_F\}, H_G\}(z) > 0$$

## Classification of singular extremals

$M = H_F$  : constant value

- $M = 0$  : **Exceptional case**
- $M > 0$  :  $\{\{H_G, H_F\}, H_G\}(z) > 0$  : **Hyperbolic case (fast)**
- $M > 0$  :  $\{\{H_G, H_F\}, H_G\}(z) < 0$  : **Elliptic case (slow)**

## Classification of regular extremals (Ekeland - IHES, Kupka - TAMS)

Denote :

- $\sigma_+$  : bang arc with  $u = +1$
- $\sigma_-$  : bang arc with  $u = -1$
- $\sigma_s$  : singular arc  $u = u_s \in ]-1, 1[$

$\sigma_1\sigma_2$  is the arc  $\sigma_1$  followed by  $\sigma_2$ .

## Classification of regular extremals (Ekeland - IHES, Kupka - TAMS)

Denote :

- $\sigma_+$  : bang arc with  $u = +1$
- $\sigma_-$  : bang arc with  $u = -1$
- $\sigma_s$  : singular arc  $u = u_s \in ]-1, 1[$

$\sigma_1\sigma_2$  is the arc  $\sigma_1$  followed by  $\sigma_2$ .

### Switching surface :

- $\Sigma : \{(q, p) \mid p \cdot G(q) = 0\}$
- $\Sigma' : \{(q, p) \mid p \cdot G(q) = p \cdot [G, F](q) = 0\} \subset \Sigma$



## Classification of regular extremals (Ekeland - IHES, Kupka - TAMS)

Denote :

- $\sigma_+$  : bang arc with  $u = +1$
- $\sigma_-$  : bang arc with  $u = -1$
- $\sigma_s$  : singular arc  $u = u_s \in ]-1, 1[$

$\sigma_1\sigma_2$  is the arc  $\sigma_1$  followed by  $\sigma_2$ .

### Switching surface :

- $\Sigma : \{(q, p) \mid p \cdot G(q) = 0\}$
- $\Sigma' : \{(q, p) \mid p \cdot G(q) = p \cdot [G, F](q) = 0\} \subset \Sigma$

$\Phi(t) = p(t) \cdot G(\mathbf{q}(t))$  is the **switching function**.

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

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

Let  $t$  be a switching time.

**Ordinary Switching time** :  $t \in ]0, t_f[$  such that  $\Phi(t) = 0$  and  $\dot{\Phi}(t) \neq 0$

Lemma

*Near  $z(t)$  every extremal solution projects onto  $\sigma_+\sigma_-$  if  $\dot{\Phi}(t) < 0$  and  $\sigma_-\sigma_+$  if  $\dot{\Phi}(t) > 0$*

Let  $t$  be a switching time.

**Ordinary Switching time** :  $t \in ]0, t_f[$  such that  $\Phi(t) = 0$  and  $\dot{\Phi}(t) \neq 0$

Lemma

*Near  $z(t)$  every extremal solution projects onto  $\sigma_+\sigma_-$  if  $\dot{\Phi}(t) < 0$  and  $\sigma_-\sigma_+$  if  $\dot{\Phi}(t) > 0$*

**Fold case** : If  $\Phi(t) = \dot{\Phi}(t) = 0$  then  $z(t) \in \Sigma'$

$$\ddot{\Phi}_\varepsilon(z(t)) = p(t) \cdot ([G, F], F)(\mathbf{q}(t)) + \varepsilon ([G, F], G)(\mathbf{q}(t)), \quad \varepsilon = \pm 1$$

Let  $t$  be a switching time.

**Ordinary Switching time** :  $t \in ]0, t_f[$  such that  $\Phi(t) = 0$  and  $\dot{\Phi}(t) \neq 0$

### Lemma

Near  $z(t)$  every extremal solution projects onto  $\sigma_+\sigma_-$  if  $\dot{\Phi}(t) < 0$  and  $\sigma_-\sigma_+$  if  $\dot{\Phi}(t) > 0$

**Fold case** : If  $\Phi(t) = \dot{\Phi}(t) = 0$  then  $z(t) \in \Sigma'$

$$\ddot{\Phi}_\varepsilon(z(t)) = p(t) \cdot ([G, F], F)(\mathbf{q}(t)) + \varepsilon [G, F], G(\mathbf{q}(t)), \quad \varepsilon = \pm 1$$

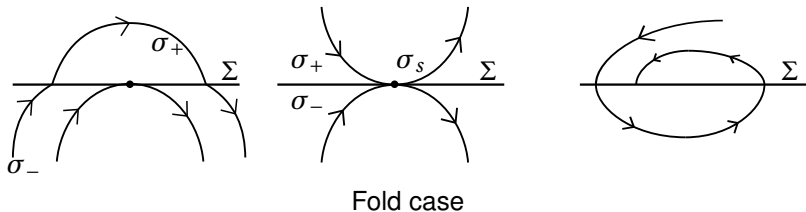
*Assumption* :  $\Sigma'$  : surface of codimension two,  $\ddot{\Phi}_\varepsilon(z(t)) \neq 0$  for  $\varepsilon = \pm 1$ .

$z(t)$  : fold point

- **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  $\ddot{\Phi}_-(t) > 0$

$u_s$  is the singular control defined by

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



In the parabolic case  $|u_0| > 1$  and the singular arc is not admissible.

### Theorem (Kupka TAMS)

In the neighborhood of  $z(t)$  every extremals projects onto :

- *Parabolic case* :  $\sigma_+ \sigma_- \sigma_+$  or  $\sigma_- \sigma_+ \sigma_-$
- *Hyperbolic case* :  $\sigma_{\pm} \sigma_s \sigma_{\pm}$
- *Elliptic case* : every extremal is of the form  $\sigma_+ \sigma_- \sigma_+ \sigma_- \dots$  (Bang-Bang) but the number of switches is not uniformly bounded.

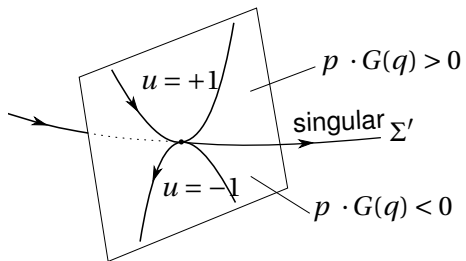


FIGURE – Fold case in the hyperbolic case and the turnpike phenomenon

# **Application to Chemical Networks**

## Time minimal synthesis for chemical systems

$$\left\{ \begin{array}{l} \min t_f \quad |u| \leq 1 \\ \dot{\mathbf{q}} = F(\mathbf{q}) + u G(\mathbf{q}) \\ \mathbf{c}_1(t_f) \in \mathbf{N} = \{\mathbf{c}_1 = d\} \end{array} \right.$$

*Methods* : Two steps :

- ① Calculation of the time minimal syntheses near the terminal manifold

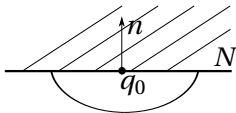


## Time minimal synthesis for chemical systems

$$\left\{ \begin{array}{l} \min t_f \quad |u| \leq 1 \\ \dot{\mathbf{q}} = F(\mathbf{q}) + u G(\mathbf{q}) \\ \mathbf{c}_1(t_f) \in \mathbf{N} = \{\mathbf{c}_1 = d\} \end{array} \right.$$

*Methods* : Two steps :

- ① Calculation of the time minimal syntheses near the terminal manifold
- ② Bounds on the number of switches

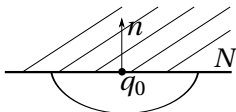


## Time minimal synthesis for chemical systems

$$\left\{ \begin{array}{l} \min t_f \quad |u| \leq 1 \\ \dot{\mathbf{q}} = F(\mathbf{q}) + u G(\mathbf{q}) \\ \mathbf{c}_1(t_f) \in \mathbf{N} = \{\mathbf{c}_1 = d\} \end{array} \right.$$

*Methods* : Two steps :

- ① Calculation of the time minimal syntheses near the terminal manifold
- ② Bounds on the number of switches



Step 1: Take  $q_0 \in \mathbf{N}$ ,  $z_0 = (q_0, n(q_0))$  where  $n(q_0)$  is the normal vector of  $\mathbf{N}$  at  $q_0$ .

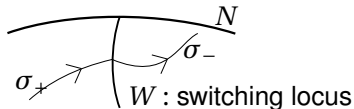
Find, in a small neighborhood  $U$  of  $q_0$ , the time minimal closed loop control  $u^*(q)$  to reach  $\mathbf{N}$  starting from  $\mathbf{q}$  in minimal time.

**Computations** :  $\dot{\mathbf{q}} = F(\mathbf{q}) + uG(\mathbf{q}), \mathbf{q}(t_f) \in \mathbf{N}$

*Synthesis* : it means

- determine the **switching locus**

Ex. :

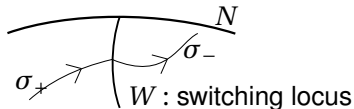


**Computations** :  $\dot{\mathbf{q}} = F(\mathbf{q}) + uG(\mathbf{q}), \mathbf{q}(t_f) \in \mathbf{N}$

*Synthesis* : it means

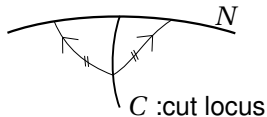
- determine the **switching locus**

Ex. :



- determine the **splitting locus** or the **cut locus**  $C$  where two distinct optimal trajectories occur.

Ex. :



**Tools** : Singularity theory  $\mathbf{N} = \{f^{-1}(0)\}$

- *expand* at  $q_0$  with Taylor series : jet spaces.
- *compute* : Normal form to estimate  $W, C$  near  $q_0$ . Tools are simple but the classification is complicated.

**Tools** : Singularity theory  $\mathbf{N} = \{f^{-1}(0)\}$

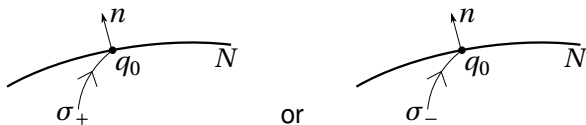
- *expand* at  $q_0$  with Taylor series : jet spaces.
- *compute* : Normal form to estimate  $W, C$  near  $q_0$ . Tools are simple but the classification is complicated.

Ex. : *Two reactions only.*  $(c, T) \in \mathbb{R}^3$ ,  $\dot{\mathbf{q}} = F + uG$  and  $\mathbf{N} = f^{-1}(0)$ .

**Generic case**  $z_0 = (q_0, n(q_0))$ .

**G is tangent to N** : Then  $p \cdot G = 0$  so  $p$  is normal to  $\mathbf{N}$ .

Using classification of extremals at a point such that  $p \cdot G(\mathbf{q}) = 0$ ,  
 $p \cdot [G, F](\mathbf{q}) \neq 0$  :



depending on the sign of  $p \cdot [G, F](q_0)$ .

... but there are more complicated situations

Define :

$\mathcal{S}$  the singular locus :  $\{\mathbf{q} \in \mathbf{N}; n \cdot [G, F](\mathbf{q}) = 0\}$

$\mathcal{E}$  the exceptional locus :  $\{\mathbf{q} \in \mathbf{N}; n \cdot F(\mathbf{q}) = 0\}$

Define :

$\mathcal{S}$  the singular locus :  $\{\mathbf{q} \in \mathbf{N}; n \cdot [G, F](\mathbf{q}) = 0\}$

$\mathcal{E}$  the exceptional locus :  $\{\mathbf{q} \in \mathbf{N}; n \cdot F(\mathbf{q}) = 0\}$

For  $\mathcal{S}$  : from the classification near a fold point one has :

- *Hyperbolic* case
- **Elliptic** case
- *Parabolic* case



Define :

$\mathcal{S}$  the singular locus :  $\{\mathbf{q} \in \mathbf{N}; n \cdot [G, F](\mathbf{q}) = 0\}$

$\mathcal{E}$  the exceptional locus :  $\{\mathbf{q} \in \mathbf{N}; n \cdot F(\mathbf{q}) = 0\}$

For  $\mathcal{S}$  : from the classification near a fold point one has :

- *Hyperbolic* case
- *Elliptic* case
- *Parabolic* case

To make the analysis we construct a semi-normal form :  $\mathbf{q} = (x, y, z)$  near 0

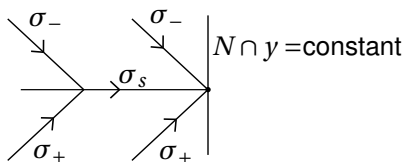
$$\begin{cases} \dot{x} = 1 + a(x) z^2 + 2b(x) yz + c(x) y^2 + \dots \\ \dot{y} = d(x) y + e(0) + \dots \\ \dot{z} = (u - \hat{u}(x)) + f(x)y + g(0)z + \dots \end{cases}$$

with

- $\mathbf{N}$  is identified to  $x = 0$
- the singular arc is identified to  $\sigma_s : t \rightarrow (t, 0, 0)$  with singular control  $\hat{u}$ .
- $a(0) < 0$  : hyperbolic if  $|\hat{u}| < 1$ .
- $a(0) > 0$  : elliptic if  $|\hat{u}| < 1$ .
- parabolic if  $|\hat{u}| > 1$ .

*Synthesis* : There exists a  $C^0$ -foliation by planes such that in each plane the synthesis is :

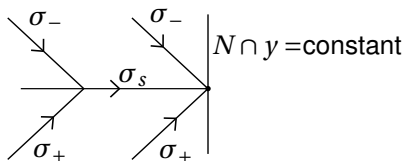
Case : Hyperbolic.



Note that the synthesis is  $\sigma_{\pm}\sigma_s\sigma_{\pm}$  hence the temperature is not constant.

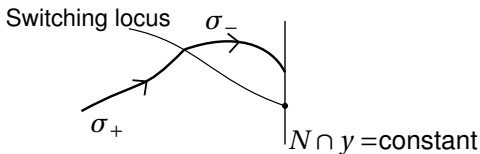
*Synthesis* : There exists a  $C^0$ -foliation by planes such that in each plane the synthesis is :

Case : Hyperbolic.

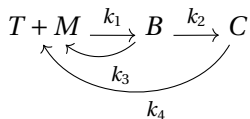


Note that the synthesis is  $\sigma_{\pm}\sigma_s\sigma_{\pm}$  hence the temperature is not constant.

Case : Parabolic. For instance, a synthesis is



# The McKeithan network



Stratification of the terminal manifold :

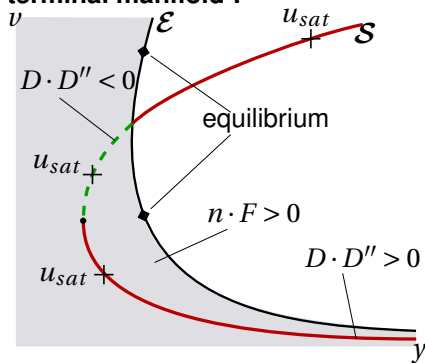


FIGURE – Dotted line : elliptic, red line : hyperbolic.

# Bridge phenomenon

**Local (planar) simplified model** (inspired from the saturation problem in Magnetic Resonance Imaging) :

$$\min_{u(\cdot)} t_f \quad \dot{q}(t) = F(q(t)) + u G(q(t)), \quad t \in [0, t_f]$$

where

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

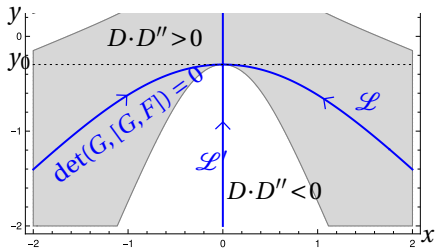
**Singular lines**  $\mathcal{L} : \det(G, [G, F])(q) = 0$

- **fast** if  $D(q) \cdot D''(q) > 0$
- **slow** if  $D(q) \cdot D''(q) < 0$

where  $D(q) = \det(G(q), [G, F](q), [[G, F], G](q))$

and  $D'(q) = \det(G(q), [G, F](q), [[G, F], F](q))$

## Singular sets

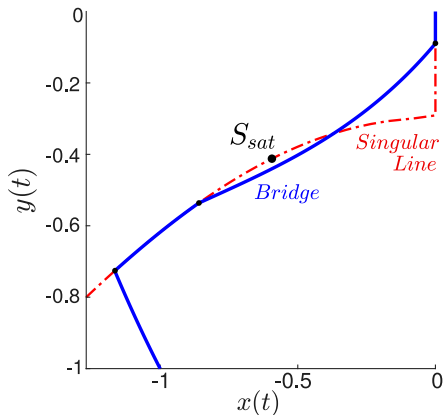


The **Singular control** along  $\mathcal{L}$  is

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

and is not bounded.

## Trajectories : bridge



Bridge connecting two switching points of the singular set.

# Conclusion

General techniques to handle complicated networks.

Even a simple network  $A \rightarrow B \rightarrow C$  can give complex optimal solution : work in progress on the *McKeithan network*. **Geometric approach** : Find coordinates to analyze the syntheses

→ applicable to general networks



# Conclusion

General techniques to handle complicated networks.

Even a simple network  $A \rightarrow B \rightarrow C$  can give complex optimal solution : work in progress on the *McKeithan network*. **Geometric approach** : Find coordinates to analyze the syntheses  
→ applicable to general networks

## Details :

B. Bonnard, J. Rouot, *Geometric Techniques to Optimize the Yield of Chemical Reactors by Temperature Control with Application to the McKeithan Network* (submitted 2019)

T. Bakir, B. Bonnard, J. Rouot, *Geometric Optimal Control Techniques to Optimize the Production of Chemical Reactors using Temperature Control*  
Annual Reviews in Control, Elsevier, **48** (2019) pp.178–192.

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.