Optimization of chemical batch reactors using temperature control

Jérémy Rouot, Bernard Bonnard

Optimization of chemical batch reactors using temperature control

Jérémy Rouot

ISEN, Brest, France

58th Conference on Decision and Control
Nice, France
December 11th–13th 2019

joint work with B. Bonnard (INRIA & UBFC)

Chemical Networks with mass action kinetics

Graph Model :

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

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

$$\underbrace{\sum_{i=1}^{m} \alpha_i X_i}_{y} \longrightarrow \underbrace{\sum_{i=1}^{m} \beta_i X_i}_{y'}$$

α_i, β_i are the stoichiometric coefficients.

Chemical Networks with mass action kinetics

Graph Model :

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

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

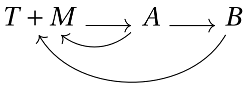
$$\underbrace{\sum_{i=1}^{m} \alpha_i X_i}_{y} \longrightarrow \underbrace{\sum_{i=1}^{m} \beta_i X_i}_{y'}$$

α_i, β_i are the stoichiometric coefficients.

Feinberg-Horn-Jackson graph

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

ex :



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

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

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

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

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

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

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

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

Dynamics for the network

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

The dynamics is defined by the graph.

Dynamics for the network

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

The dynamics is defined by the graph.

- **Stoichiometric subspace**

$$S = \mathbf{span}\left\{\mathbf{y}-\mathbf{y}', \mathbf{y}\to\mathbf{y}' \in \mathscr{R}\right\}$$

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

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

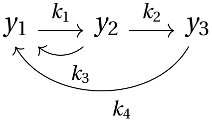
Lemma

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

Notations

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

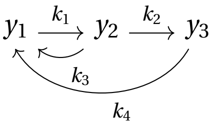
ex :



Notations

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

ex :

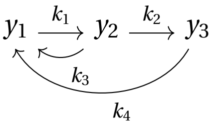


- **Complex matrix :** $Y = (y_1, \ldots, y_n)$ (n : number of vertices).

Notations

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

ex :

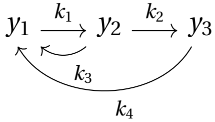


- **Complex matrix :** $Y = (y_1, \ldots, y_n)$ (n : number of vertices).
- **Incidence connectivity matrix :** $\boldsymbol{A = (a_{ij})_{ij}}$
  with for instance $a_{21} = k_1$ indicating a reaction with constant k_1 from the first node of the graph to the second : $y_1 \xrightarrow[k_1]{} y_2$

Notations

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

ex :



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

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

One has

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

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

Zero deficiency theorem

Definition (Deficiency)

Feinberg and Horn-Jackson : articles in Archive Rational Mechanics
Graph concept : *deficiency :* $\boldsymbol{\delta = n - l - s}$ *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 $\boldsymbol{\delta = 0}$ *(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* $V(c,c^*) = \sum_i \left[c_i(\ln(c_i) - \ln(c_i^*) - 1) + c_i^*\right]$.
   Moreover there are no non trivial periodic orbits.

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

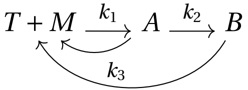
Theorem

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* $V(c,c^*) = \sum_i \left[c_i(\ln(c_i) - \ln(c_i^*) - 1) + c_i^*\right]$.
   Moreover there are no non trivial periodic orbits.

Application : Test bed cases :

case 1 : $A \xrightarrow{k_1} B \xrightarrow{k_2} C$ $\qquad \delta = 3 - 1 - 2 = 0$: not weakly reversible

case 2 : (**McKeithan network)**



$\delta = 3 - 1 - 2 = 0$: one single equilibirum globally asymptotically stable

Equilibrium for the McKeithan network

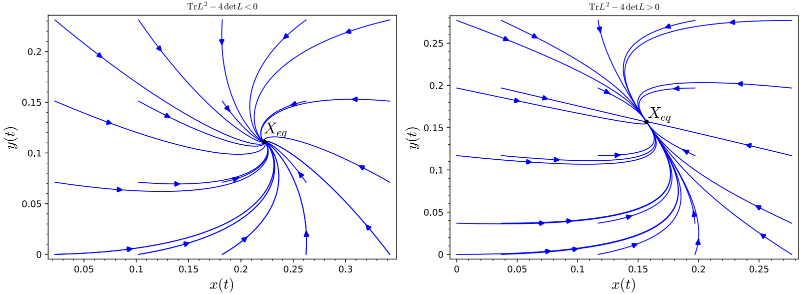


FIGURE – Phase portrait for the McKeithan model. (left) Focus ; (right) Node.

Geometric Optimal Control

Optimal Control Problem

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

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

Single input C^ω-control system, affine in u :

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

Formulation :

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

Formulation :

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

Formulated as

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

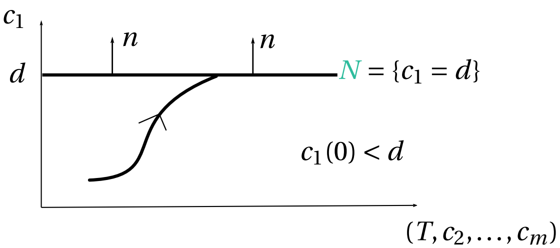
Formulation :

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

Formulated as

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

$\mathbf{N}$: terminal manifold of codimension 1.



Necessary optimality conditions Pontryagin Maximum Principle (1956)

Notations :

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

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

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

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* $[0, t_f^*]$ *:*

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

the maximization condition is satisfied

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

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* $[0, t_f^*]$ *:*

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

the maximization condition is satisfied

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

Moreover

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

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

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

$$\frac{\mathrm{d}}{\mathrm{d}t} H_G(z) = \mathrm{d}H_G \cdot \dot{z} = \{H_G, H_F + u\,H_G\} = \mathbf{\{H_G, H_F\} = 0}$$

$$\mathbf{\{\{H_G, H_F\}, H_F\}(z) + u\,\{\{H_G, H_F\}, H_G\}(z) = 0}$$

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

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

$\Rightarrow$ 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 :

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

$\sigma_1\sigma_2$ is the arc σ_1 followed by σ_2.

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

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

$\sigma_1\sigma_2$ is the arc σ_1 followed by σ_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 :

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

$\sigma_1\sigma_2$ is the arc σ_1 followed by σ_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**.
$\dot{\Phi}(t) = p(t) \cdot [G,F](\mathbf{q(t)})$
$\ddot{\Phi}(t) = p(t) \cdot \big([[G,F],F](\mathbf{q(t)}) + u(t)\,[[G,F],G](\mathbf{q(t)})\big)$

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 $z(t) \in \Sigma'$

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

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 $z(t) \in \Sigma'$

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

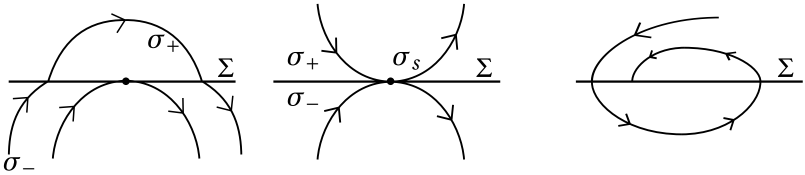
Assumption : Σ' : surface of codimension two, $\ddot{\Phi}_\varepsilon(z(t)) \neq 0$ for $\varepsilon = \pm 1$.

$z(t)$: 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

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



Fold case

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 $\sigma_+\sigma_-\sigma_+\sigma_-\ldots$ (Bang-Bang) but the number of switches is not uniformly bounded.*

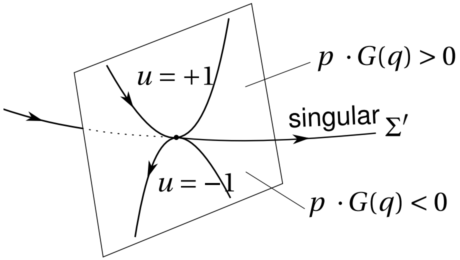


FIGURE – Fold case in the hyperbolic case and the turnpike phenomenon

Application to Chemical Networks

Time minimal synthesis for chemical systems

$$\begin{cases} \min\ t_f \qquad |u| \le 1 \\ \dot{\mathbf{q}} = F(\mathbf{q}) + u\,G(\mathbf{q}) \\ \mathbf{c_1}(t_f) \in \mathbf{N} = \{\mathbf{c_1} = d\} \end{cases}$$

Methods : Two steps :

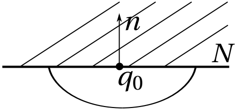
1. Calculation of the time minimal syntheses near the terminal manifold

Time minimal synthesis for chemical systems

$$\begin{cases} \min\ t_f \qquad |u| \le 1 \\ \dot{\mathbf{q}} = F(\mathbf{q}) + u\,G(\mathbf{q}) \\ \mathbf{c_1}(t_f) \in \mathbf{N} = \{\mathbf{c_1} = d\} \end{cases}$$

Methods : Two steps :

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

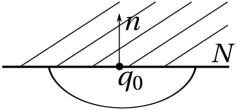


Time minimal synthesis for chemical systems

$$\begin{cases} \min\ t_f \qquad |u| \leq 1 \\ \dot{\mathbf{q}} = F(\mathbf{q}) + u\,G(\mathbf{q}) \\ \mathbf{c_1}(t_f) \in \mathbf{N} = \{\mathbf{c_1} = d\} \end{cases}$$

Methods : Two steps :

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



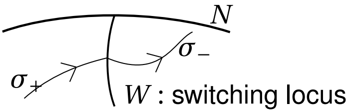
`Step 1`: Take $q_0 \in \mathbf{N}$, $z_0 = (q_0, n(q_0))$ where $n(q_0)$ is the normal vector of $\mathbf{N}$ at q_0.
Find, in a small neighborhood U of q_0, the time minimal closed loop control $u^*(q)$ to reach $\mathbf{N}$ starting from $\mathbf{q}$ in minimal time.

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

Synthesis : it means

- determine the **switching locus**

  Ex. :

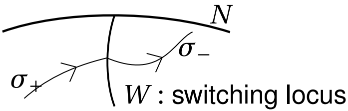


Computations : $\dot{\mathbf{q}} = F(\mathbf{q}) + u\,G(\mathbf{q}),\; q(t_f) \in \mathbf{N}$

Synthesis : it means

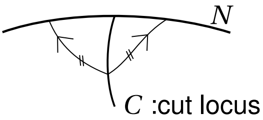
- determine the **switching locus**

  Ex. :



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

  Ex. :



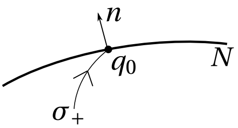
Tools : Singularity theory $\mathbf{N} = \{f^{-1}(0)\}$

- *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.

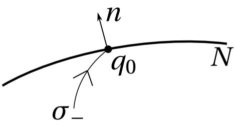
Tools : Singularity theory $\mathbf{N} = \{f^{-1}(0)\}$

- *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*. $(c, T) \in \mathbb{R}^3$, $\dot{\mathbf{q}} = F + u\,G$ and $\mathbf{N} = f^{-1}(0)$.
Generic case $z_0 = (q_0, n(q_0))$.
***G* is tangent to $\mathbf{N}$** : Then $p \cdot G = 0$ so p is normal to $\mathbf{N}$.
Using classification of extremals at a point such that $p \cdot G(\mathbf{q}) = 0$,
$p \cdot [G, F](\mathbf{q}) \neq 0$:



or



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

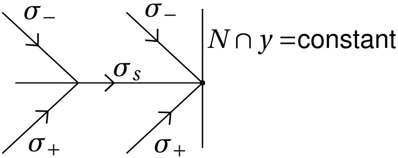
$$\begin{cases} \dot{x} = 1 + a(x)\, z^2 + 2b(x)\, yz + c(x)\, y^2 + \dots \\ \dot{y} = d(x)\, y + e(0) + \dots \\ \dot{z} = (u - \hat{u}(x)) + f(x)\, y + g(0)\, z + \dots \end{cases}$$

with

- $\mathbf{N}$ is identified to $x = 0$
- the singular arc is identified to $\sigma_s : t \to (t, 0, 0)$ 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 :

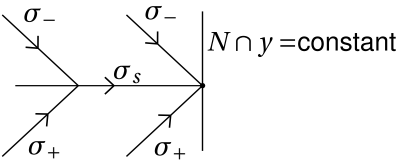
Case : Hyperbolic.



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

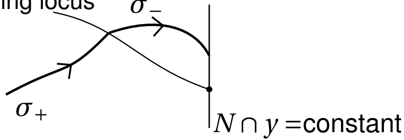
Synthesis : There exists a C^0-foliation by planes such that in each plane the synthesis is :

Case : Hyperbolic.

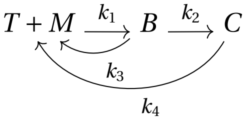


Note that the synthesis is $\sigma_\pm \sigma_s \sigma_\pm$ hence the temperature is not constant.

Case : Parabolic. For instance, a synthesis is



The McKeithan network



Stratification of the terminal manifold :

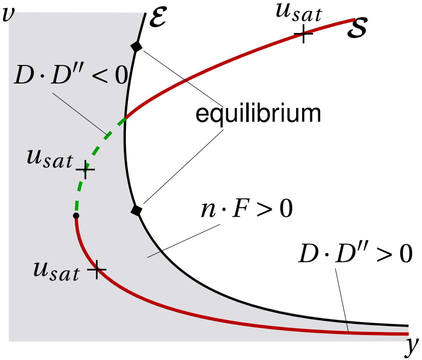


FIGURE – Dotted line : elliptic, red line : hyperbolic.

Bridge phenomenon

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

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

where

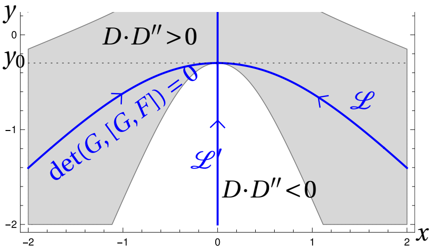
$$q = (x, y), \quad F = (1 - x^2 y)\frac{\partial}{\partial y}, \quad G = -(y-1)\frac{\partial}{\partial x} + x\frac{\partial}{\partial y}.$$

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

- **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

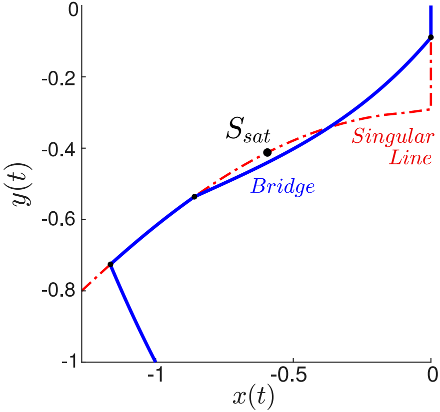


The **Singular control** along $\mathscr{L}$ is

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

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 $A \to B \to C$ 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 $A \to B \to C$ 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.