Optimization of chemical batch reactors using temperature control

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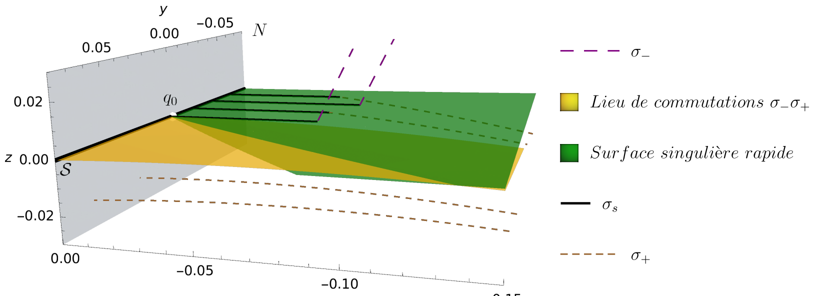
joint work with B. Bonnard (INRIA & UBFC)

Problem :

- Analytic control sytem : $\dot{q}(t) = X(q(t)) + u(t)Y(q(t))$
- State $q = (x, y, z) \in \mathbb{R}^3$, $u \in [-1, 1]$,
- Reach a terminal manifold **N** of codimension 1 in minimum time

Aim :

- Classification of generic (local) synthesis. Related to the singularities of the solutions of Hamilton-Jacobi-Bellman equation
- Approximate subanalytic singularity sets by semi-algebraic sets (normal forms)
- Compute optimal control in closed loop : Motivated by chemical networks optimization



Context : Chemical Network

Graph Model :

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

Notations : $\mathscr{R}$ is the set of reactions of the form : $\mathbf{y} \rightarrow \mathbf{y}'$

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

α_i, β_i are the stoichiometric coefficients.

Chemical Networks with mass action kinetics

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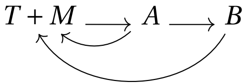
Feinberg-Horn-Jackson graph

- Vertices : $\mathbf{y} = (\alpha_\mathbf{1}, \ldots, \alpha_\mathbf{m})^\top$, $\mathbf{y}' = (\beta_\mathbf{1}, \ldots, \beta_\mathbf{m})^\top$
- 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

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  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

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

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- **Stoichiometric subspace**

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

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

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

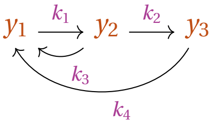
Lemma

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 :



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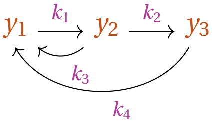

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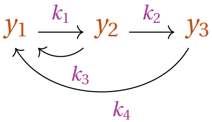

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  with for instance $a_{21} = k_1$ indicating a reaction with constant k_1 from the first node of the graph to the second : $y_1 \xrightarrow[k_1]{} y_2$

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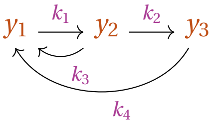

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- **Laplacian matrix :**

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

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 $\delta = 0$ *(Zero deficiency assumption)*

Theorem (Feinberg-Horn-Jackson (1970s))

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.

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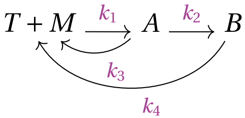
Application : Test bed cases :

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

case 2 : (**McKeithan network)**



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

Equilibrium for the McKeithan network

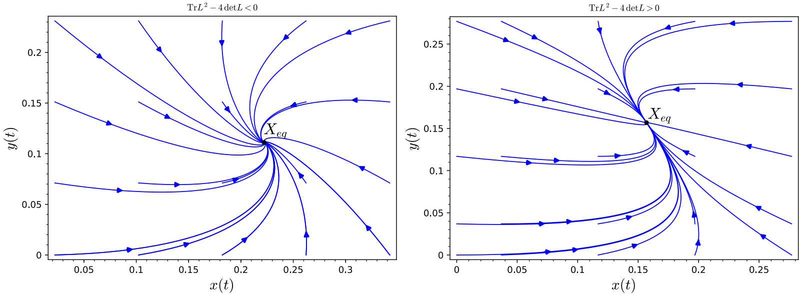


FIGURE – Phase portrait for the McKeithan model. (left) Focus ; (right) Node.

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

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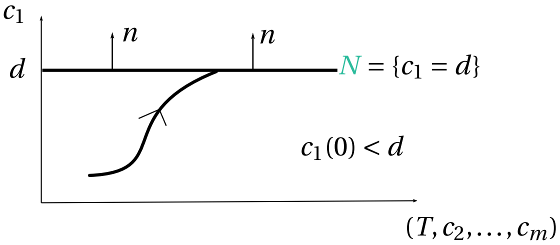
N : terminal manifold of codimension 1.



Necessary optimality conditions Pontryagin Maximum Principle (1956)

Notations :

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

- $H(\mathbf{q}, p, u) = p \cdot (F(\mathbf{q}) + u\,G(\mathbf{q})),\ p \in \mathbb{R}^n \setminus \{0\}$: 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 (Pontryagin et al. 1956)

Assume $(q^*(\cdot), u^*(\cdot))$ *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

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

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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 :

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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

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

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

Strict generalized Legendre-Clebsch condition

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

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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.

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Switching surface :

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

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

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

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

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* $\dot{\Phi}(t) > 0$

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Lemma

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

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

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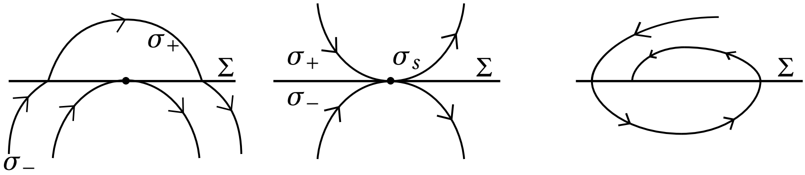
Assumption : Σ' : surface of codimension two, $\ddot{\Phi}_\varepsilon(z(t)) \neq 0$ for $\varepsilon = \pm 1$.

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



Parabolic, Hyperbolic, Fold case, Elliptic

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

Theorem (Kupka, 1987 (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.*

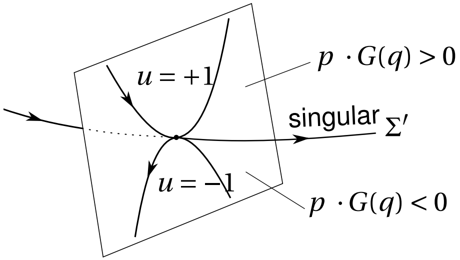


FIGURE – Fold case in the hyperbolic case and the turnpike phenomenon

Application to Chemical Networks

Time minimal synthesis for chemical systems

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

Methods : Two steps :

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

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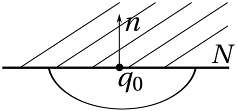

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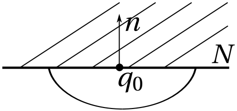


`Step 1`: Take $q_0 \in \mathbf{N}$, $z_0 = (q_0, n(q_0))$ where $n(q_0)$ is the normal vector of $\mathbf{N}$ at q_0.

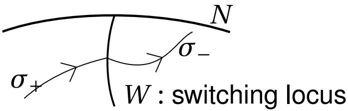
Find, in a small neighborhood U of q_0, the time minimal closed loop control $u^*(q)$ to reach $\mathbf{N}$ starting from $\mathbf{q}$ in minimal time.

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. :



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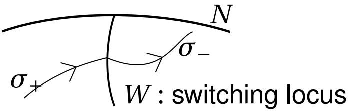

- determine the **splitting locus** or the **cut locus** C where two distinct optimal trajectories occur.

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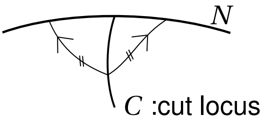

Tools : Singularity theory $\mathbf{N} = \{f^{-1}(0)\}$

- *expand* at q_0 with Taylor series : jet spaces.
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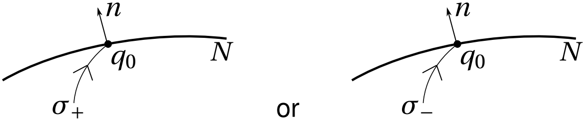
Ex. : *Two reactions only*. $(c, T) \in \mathbb{R}^3$, $\dot{\mathbf{q}} = F + u\,G$ and $\mathbf{N} = f^{-1}(0)$.

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

***G* is tangent to 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 : $\{\mathbf{q} \in \mathbf{N};\ n \cdot F(\mathbf{q}) = 0\}$

Stratification of the terminal manifold :

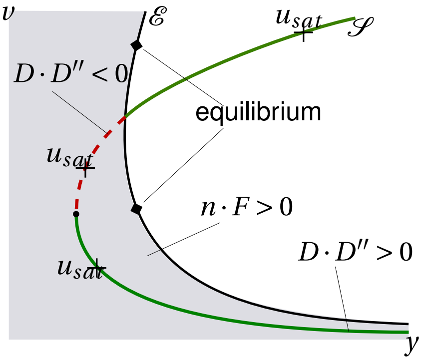


FIGURE – Dotted line : elliptic, red line : hyperbolic.

Define :

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

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

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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

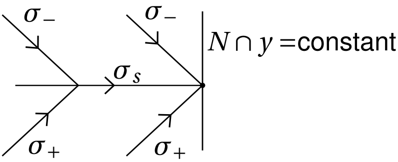
$$\begin{cases} \dot{x} = 1 + a(x)\, z^2 + 2b(x)\, yz + c(x)\, y^2 + \dots \\ \dot{y} = d(x)\, y + e(0) + \dots \\ \dot{z} = (u - \hat{u}(x)) + f(x)\, y + g(0)\, z + \dots \end{cases}$$

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.

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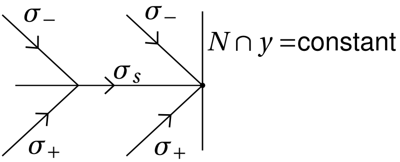
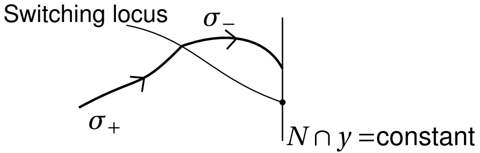
Case : Hyperbolic.

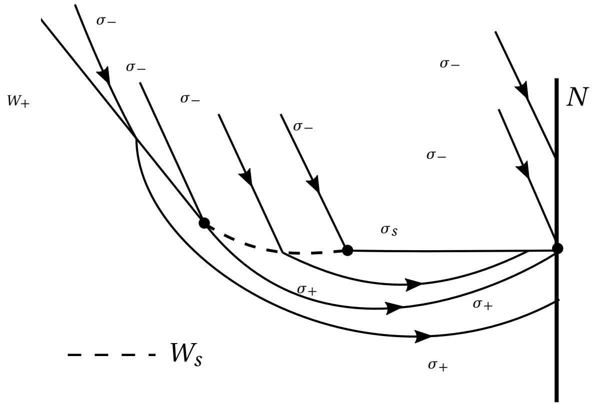


Note that the synthesis is $\sigma_\pm \sigma_s \sigma_\pm$ hence the temperature is not constant.

Case : Parabolic. For instance, a synthesis is



Other synthesis example



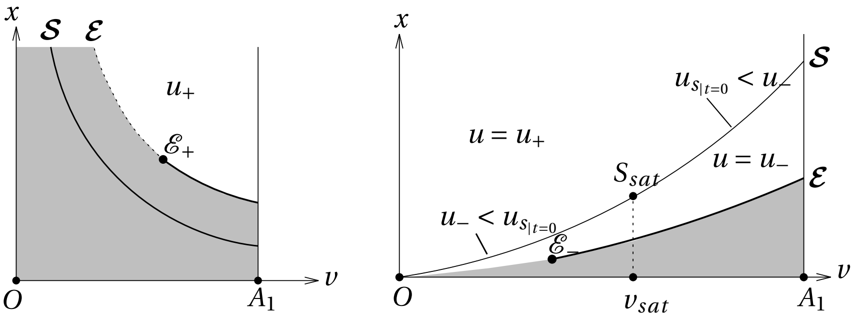
Two examples of reactions

The irreversible case

Application (non trivial) :

$$A \xrightarrow{k_1} B \xrightarrow{k_2} C$$

$\mathbf{c_1}$: concentration of A,
c_2 : concentration of B,
Final target : $\mathbf{c_1 = \boldsymbol{d}}$
Parameter $\alpha = E_2/E_1$.

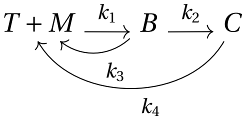


- α **< 1** : Singular arcs are not admissible : optimal policy : $u = \pm 1$.
- α **> 1** : Different cases : singular arcs are admissible and the optimal policy is $\sigma_-\sigma_s\sigma_+$.

Theorem (Bonnard, Pelletier)

Every optimal trajectory has **at most two switchings** *and of the form* $\sigma_+\sigma_-\sigma_s$ *where each arc of the sequence can be empty.*

The McKeithan network



Stratification of the terminal manifold :

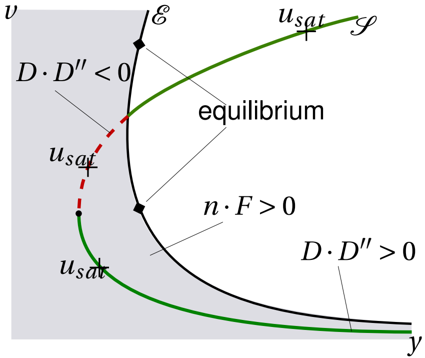


FIGURE – Dotted line : elliptic, red line : hyperbolic, $\mathbf{S}$: Singular locus.

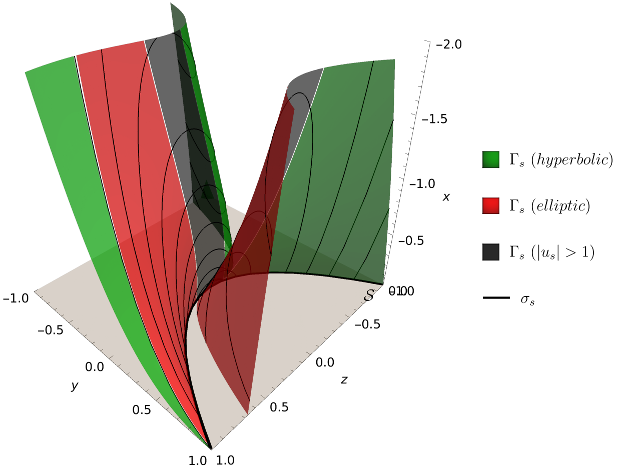


FIGURE – Singular surface foliated by singular trajectories.

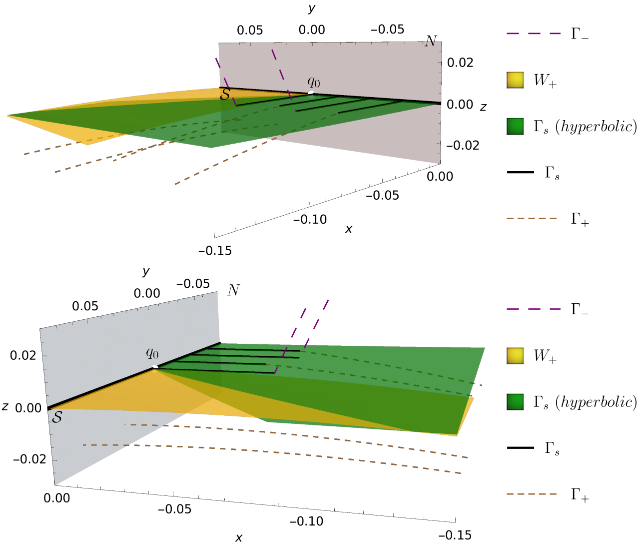
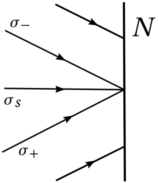
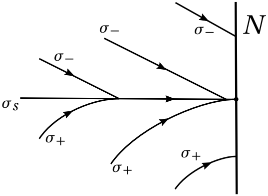


FIGURE – Local synthesis obtained via symbolic computations.



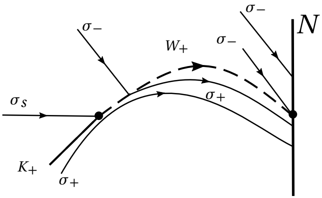
σ_-
N
σ_s
σ_+

$y < 0$



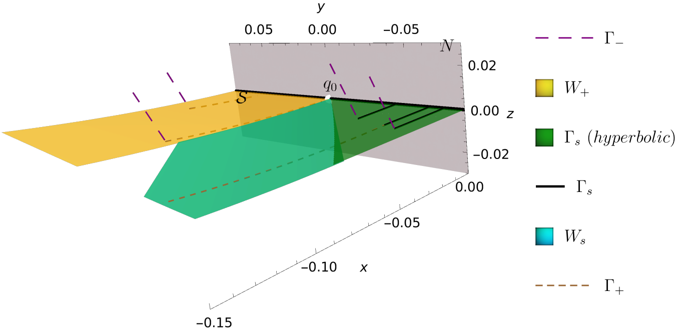
σ_-
σ_-
N
σ_-
σ_s
σ_+
σ_+
σ_+

$y = 0$



σ_-
N
σ_-
W_+
σ_-
σ_s
σ_+
K_+
σ_+

$y > 0$



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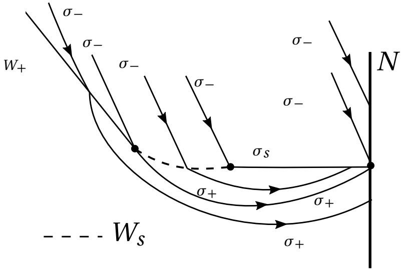
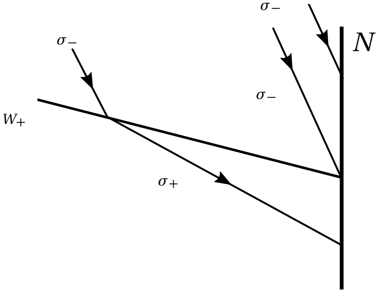

σ_-
σ_-
σ_-
σ_-
σ_-
σ_-
W_+
N
σ_s
σ_+
σ_+
σ_+
W_s

$y < 0$


σ_-
σ_-
σ_-
N
W_+
σ_+

$y > 0$

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

On-going work :

- Normal forms to investigate local synthesis near the singularity of the singular set.
- Relate to the solutions of Hamilton-Jacobi-Bellman (local to global)
- Analyze the conjugate locus

Details :

- B. Bonnard, J. Rouot, *Geometric Techniques to Optimize the Yield of Chemical Reactors by Temperature Control with Application to the McKeithan Network* (accepted 2020)
- 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.