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Optimal Control of an Ensemble of Bloch Equations with Applications in MRI.

55th IEEE Conference on Decision and Control

Bernard Bonnard, Alain Jacquemard and Jérémy Rouot

- Ensemble of spin particles: mathematical model in Nuclear Magnetic Resonance
- (Multi)Saturation problem, constraint problem
⇒ Optimal control problem (Mayer formalism)
- Geometric optimal control: Pontryagin Maximum Principle, second order optimality conditions
- Numerical methods: Direct methods (Bocop software), Indirect methods (Ham-path Software), Global methods based on SOS-moment approach (Globtipoly)

Bloch equations M_i : magnetization vector of the spin particle $i \in \{1 \dots N\}$.

$$\dot{M}_i(t) = \kappa M_i(t) \times B(t) + R(M_i)$$

- dissipative term:

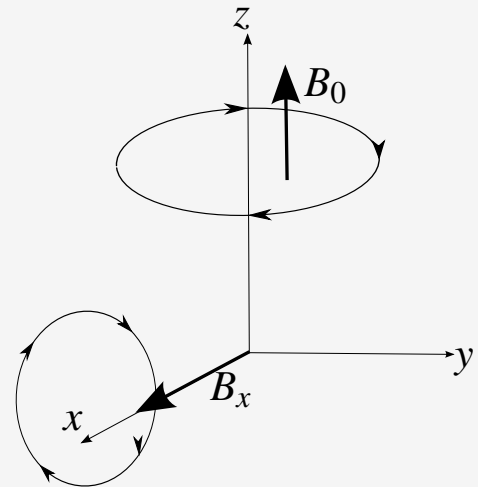
$$R(M_i) = (M_{x_i}/T_2^i, M_{y_i}/T_2^i, (M_{z_i} - M_0^i)/T_1^i)$$

- . M_0^i : equilibrium magnetization.
- . T_1^i, T_2^i : relaxation parameters, chemical signature of the species.

- $B(t) = B_0 + B_1(t)$,

- . B_0 : **strong static field.**
- . $B_1 = (B_x, B_y, 0)$: **control RF-field.**

$$u = -\kappa B_y, \quad v = -\kappa B_x, \quad u^2 + v^2 \leq m$$



Rotating frame

$$M_i(t) = S(t) q_i(t), \quad q_i = (x_i, y_i, z_i), \quad S(t) = \exp(\omega t \Omega_z), \quad \Omega_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$u_2 = u \cos(\omega t) - v \sin(\omega t), \quad u_1 = u \sin(\omega t) + v \cos(\omega t)$$

$$\frac{d}{dt} \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} = \begin{pmatrix} -1/T_2^i & -\Delta\omega_i & u_2 \\ \Delta\omega_i & -1/T_2^i & -u_1 \\ -u_2 & u_1 & -1/T_1^i \end{pmatrix} \begin{pmatrix} x_i \\ y_i \\ z_i \end{pmatrix} + \begin{pmatrix} 0 \\ 0 \\ M_0^i/T_1^i \end{pmatrix}$$

with $\Delta\omega_i$ the resonance offset.

Affine control system

$$\dot{q} = F_0(q) + u_1 F_1(q) + u_2 F_2(q), \quad q = (q_1, \dots, q_N)$$

- **saturation problem** for N spins: $\min t_f, q_i(0) = (0, 0, M_0^i), q_i(t_f) = O, i = 1, \dots, N.$
- **contrast problem** for 2 spins: $\min -|q_2(t_f)|^2, q_i(0) = (0, 0, M_0^i), i = 1, 2, q_1(t_f) = O.$

\implies Mayer problem

- system with k controls, state $q \in \mathbf{R}^n$

$$\dot{q} = F_0(q) + \sum_{i=1}^m u_i F_i(q), \quad u \in U \subset \mathbf{R}^m, \quad q(0) = q_0$$

- final boundary condition: $g(q(t_f)) = 0$
- cost to minimize: $\min_{u \in \mathcal{U}} c(q(t_f))$, $\mathcal{U} =$ admissible controls.

Necessary conditions: (q^*, u^*) optimal $\implies \exists p^* \in \mathbf{R}^n$

$$\dot{q}^* = \frac{\partial H}{\partial p}(q^*, p^*, u^*), \quad \dot{p}^* = -\frac{\partial H}{\partial q}(q^*, p^*, u^*), \quad H(q, p, u) = \langle p, F_0(q) + \sum_{i=1}^m u_i F_i(q) \rangle.$$

maximization condition:

$$H(q^*, p^*, u^*) = \max_{u \in U} H(q^*, p^*, u) = \text{constant}.$$

transversality condition:

$$p^*(t_f) = p_0 \frac{\partial c}{\partial q}(q^*(t_f)) + \sum_{i=1}^l \sigma_i \frac{\partial g_i}{\partial q}(q^*(t_f)), \quad p_0 \leq 0, \quad \sigma = (\sigma_1, \dots, \sigma_l) \in \mathbf{R}^l. \quad 5$$

Definition 1. *Extremal: solution (q, p, u) of the Hamiltonian system of the PMP.*

Define the input state mapping for (T, q_0) fixed:

$$E_{T, q_0} : u \in \mathcal{U} \mapsto q(T, q_0, u)$$

Definition 2. *u is singular on $[0, T]$ if the Fréchet derivative of E is not of full rank when evaluated at u and the corresponding trajectory $q(\cdot, q_0, u)$ is called singular on $[0, T]$.*

Symmetry of revolution along z axis: reduction to the case: $u_2 = 0$, $u_1 = u$, $M_0 = 1$, $\tau = mt$.

$\Gamma = 1/mT_2$, $\gamma = 1/mT_1$ with $2\Gamma > \gamma \rightarrow$ Bloch ball = $\{q, |q| \leq 1\}$ invariant.

$$\dot{q} = F(q) + uG(q), \quad q = (y, z), \quad |u| \leq 1$$

Definition 3. • *Regular extremal (bang):* $u = \text{sign } H_G$, $H_G = \langle p, G(q) \rangle$,

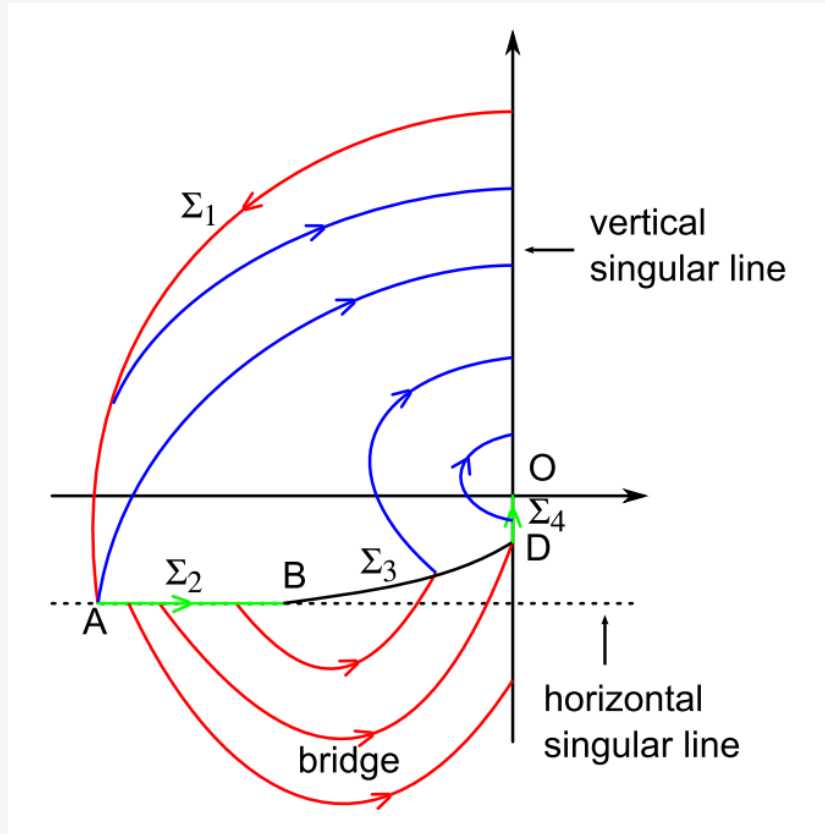
• *Singular extremal:* $H_G(q, p) = 0 \dots$

Computations of singular extremals

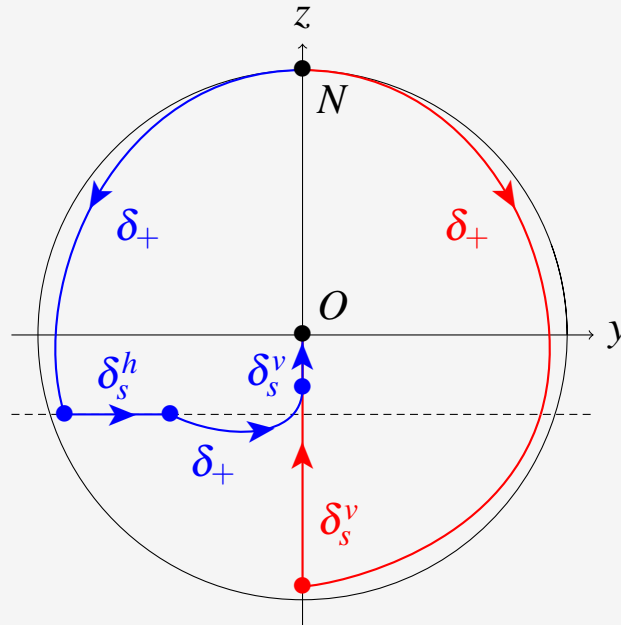
$$\begin{aligned} H_G(q, p) = 0 &\implies \{H_G, H_F\}(q, p) = 0, \\ &\implies \{\{H_G, H_F\}, H_F\}(q, p) + u_s \{\{H_G, H_F\}, H_G\}(q, p) = 0, \end{aligned}$$

$\implies u_s(\mathbf{q}, \mathbf{p})$ is defined for $(q, p) \in \Sigma_2 : H_G = \{H_G, H_F\} = 0 \setminus \{\{H_G, H_F\}, H_G\} = 0$.

Singular arcs are contained in the set $\{q, \det(G(q), [F, G](q)) = 0\}$ with an expression of $u_s(\mathbf{q})$.



Solutions for the saturation problem



Time minimal solution (left) compared with inversion sequence (right).

(left): $\tau_f = T_{\min}$, (T_{\min} known) $\rightarrow \delta_+ \delta_s^h \delta_+ \delta_s^v$

(right): Time minimal solutions: Bang-Singular: $\delta_+ \delta_s^v$

$N = 2$ spins, $(q_1, (\Gamma_1, \gamma_1)), (q_2, (\Gamma_2, \gamma_2))$.

Optimal control problem: $|u| \leq 1$.

- $q(t_f) = (0, 0)$, $q = (q_1, q_2)$,
- Mayer cost: $c(q(t_f))$,
- Dynamic: $\dot{q}_i = F_0^i(q_i) + u_1 F_1^i(q_i) + u_2 F_2^i(q_i)$, $i = 1, 2$ where

$$F_0^i = -\Gamma_i x_i \partial_{x_i} - \Gamma_i y_i \partial_{y_i} + \gamma_i (1 - z_i) \partial_{z_i},$$

$$F_1^i = -z_i \partial_{y_i} + y_i \partial_{z_i}, \quad F_2^i = z_i \partial_{x_i} - x_i \partial_{z_i}.$$

Maximization condition of the PMP. if $w = (q, p) \notin \Sigma = \{w, H_1 = H_2 = 0\}$:

$$u_j = H_j / \sqrt{H_1^2 + H_2^2}, \quad H_j = \langle p, F_j \rangle, \quad j = 1, 2$$

Singular extremals: u singular $\implies (q, p, u)$ is an extremal satisfying

$$\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}, \quad \frac{\partial H}{\partial u} = 0 \quad \text{where } H = H_0 + u_1 H_1 + u_2 H_2.$$

$$\Sigma = \Sigma_1 \cup \Sigma_2 \cup \Sigma_3$$

- If $w = (q, p) \in \Sigma_1 = \Sigma \setminus \{H_1, H_2\} = \mathbf{0}$, singular control:

$$u_s(w) = \frac{(\{H_2, H_0\}(w), \{H_0, H_1\}(w))}{\{H_1, H_2\}(w)}$$

... but it's not an admissible control $|u_s^1| > 1$.

- Goh condition: $\{H_1, H_2\} = 0$.
If $w \in \Sigma \cap \{H_1, H_2\} = 0$, then

$$\{H_0, H_1\} = \{H_2, H_0\} = 0$$

We get 3 relations that we differentiate w.r.t. the time and the singular control u_s satisfies

$$A(w) + u_s B(w) = 0$$

u_s is defined provided $w \in \Sigma_2 : H_1 = H_2 = \{H_1, H_2\} = \mathbf{0} \setminus \det \mathbf{B} = 0$.

With

$$A = \begin{pmatrix} \{\{H_0, H_1\}, H_0\} \\ \{\{H_0, H_2\}, H_0\} \end{pmatrix}, \quad B = \begin{pmatrix} \{\{H_0, H_1\}, H_1\} & \{\{H_0, H_1\}, H_2\} \\ \{\{H_0, H_2\}, H_1\} & \{\{H_0, H_2\}, H_2\} \end{pmatrix}$$

Remark 4. *It is possible to write u_s function of q only.*

$$\Sigma_3 : H_1 = H_2 = \{H_1, H_2\} = \{H_0, H_1\} = \{H_0, H_2\} = \det(\mathbf{B}) = 0$$

We can find singular extremals in Σ_3 .

- $y_2x_1 - x_2y_1$ divides $\det B$,
- $x_1 = x_2 = 0$ is invariant by the singular flow imposing $u_2 = 0$
 $\implies \det B = 0$ is forced to be invariant,
- $\{H_1, H_2\}(w) = (p_{y_1}x_1 - p_{x_1}y_1) + (p_{y_2}x_2 - p_{x_2}y_2)$ is first integral (symmetry of revolution).

Proposition 5. *The singular extremals of the single-input case with $u_2 = 0$ are extremals of the bi-input case with the additional condition: $x_1 = p_{x_1} = x_2 = p_{x_2} = 0$.*

It amounts to study the single input system

$$\dot{q} = F_0(q) + uF_1(q), \quad q = (y, z)$$

with singular control

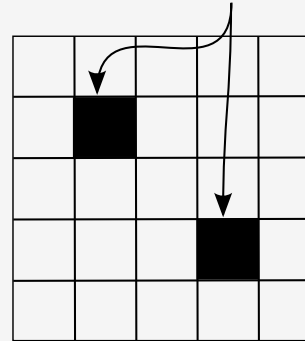
$$u_s(w) = -\frac{\{\{H_0, H_1\}, H_0\}(w)}{\{\{H_0, H_1\}, H_1\}(w)}$$

APPLICATION: MULTISATURATION OF THE SAME SPECIES WITH B_1 -INHOMOGENEITY

$q = (q_1, q_2)$, same relaxations parameters (Γ, γ) for q_1 and q_2 .

$$\begin{aligned} \min \quad & t_f \\ \text{s.t.} \quad & \dot{q}_1 = F_0(q_1) + u F_1(q_1), \\ & \dot{q}_2 = F_0(q_2) + u(\mathbf{1} - \boldsymbol{\varepsilon}) F_1(q_2), \\ & q_1(t_f) = q_2(t_f) = 0, \\ & q(0) = ((0, 1), (0, 1)). \end{aligned}$$

pixels with different B_1



Additional constraint: $H = 0$ (t_f free).

Singular control in $H_0 = H_1 = \{H_1, H_0\} = \det B = 0$:

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

$D = \det(F_0, F_1, [F_1, F_0], [[F_1, F_0], F_1])$, $D' = \det(F_0, F_1, [F_1, F_0], [[F_1, F_0], F_0])$.

\implies analysis of the flow of $F_0 - D'/DF_1$ i.e. of

$$X(q) = D(q)F_0(q) - D'(q)F_1(q)$$

Computations of the equilibrium points of X . Non trivial algebraic problem (Gröbner basis).

Theorem 6. *For $\varepsilon \neq 1$, the equilibrium points of X are all contained in $\{D(q) = 0\} \cap \{D'(q) = 0\}$.*

Proposition 7. *$\{D = 0\} \cap \{D' = 0\}$ is an algebraic variety of dimension 2 whose components are located in the hyperplane $z_1 = z_2$ and in the hypersurface $(\varepsilon - 1)z_1y_2 + z_2y_1 = 0$.*

Algebraic analysis of these components \implies computations of equilibrium points.

Further analysis: behaviours of the solutions of X near these equilibrium points using linearized methods.