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

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

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

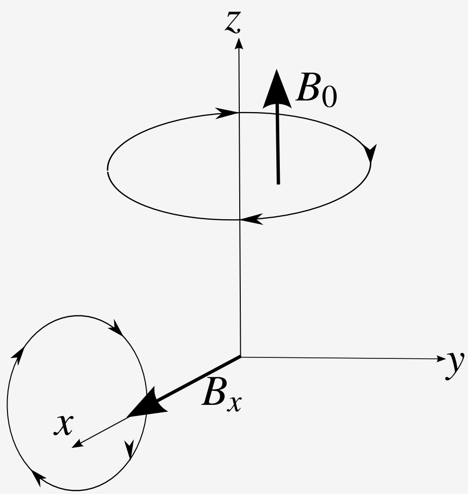
$$\dot{M}_i(t) = \kappa M_i(t) \times B(t) + R(M_i)$$

- 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 magnetizarion.

. 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**.

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

Rotating frame

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

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

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

with $\Delta\omega_i$ the resonance offset.

Affine control system

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

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

$\Longrightarrow$ 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: $\min_{u \in \mathscr{U}} c(q(t_f))$, $\mathscr{U}$ = admissible controls.

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

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

maximization condition:

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

transversality condition:

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

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

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

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

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* $q(.,q_0,u)$ *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 $2\Gamma > \gamma \to$ 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):* $u = \text{sign}\, H_G, \quad H_G = \langle p, G(q) \rangle$,

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

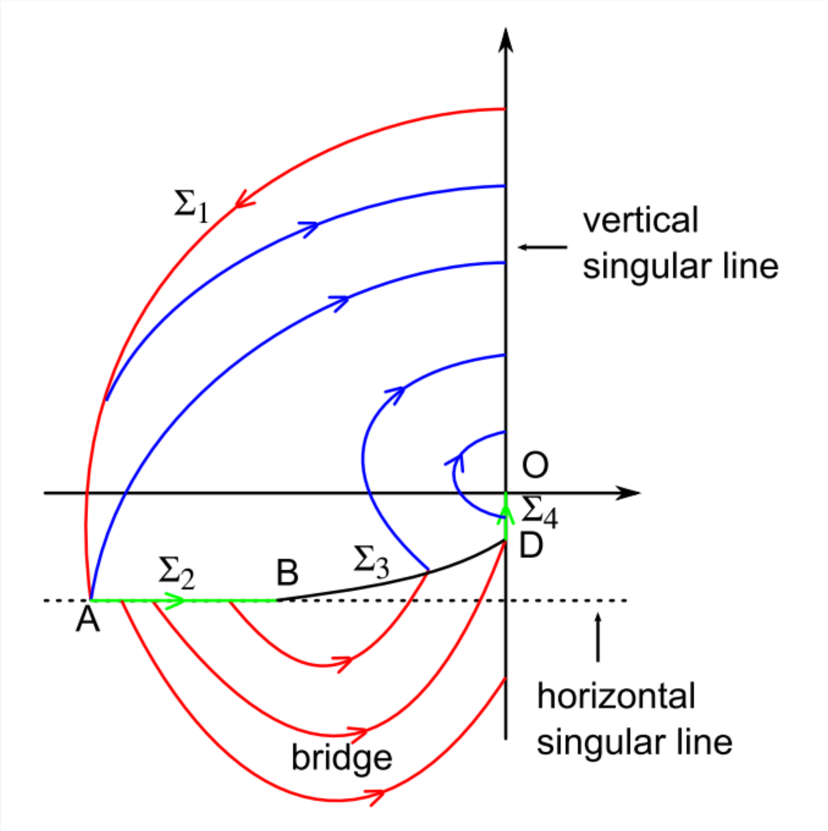
Computations of singular extremals

$$H_G(q,p) = 0 \Longrightarrow \{H_G, H_F\}(q,p) = 0,$$
$$\Longrightarrow \{\{H_G, H_F\}, H_F\}(q,p) + u_s\{\{H_G, H_F\}, H_G\}(q,p) = 0,$$

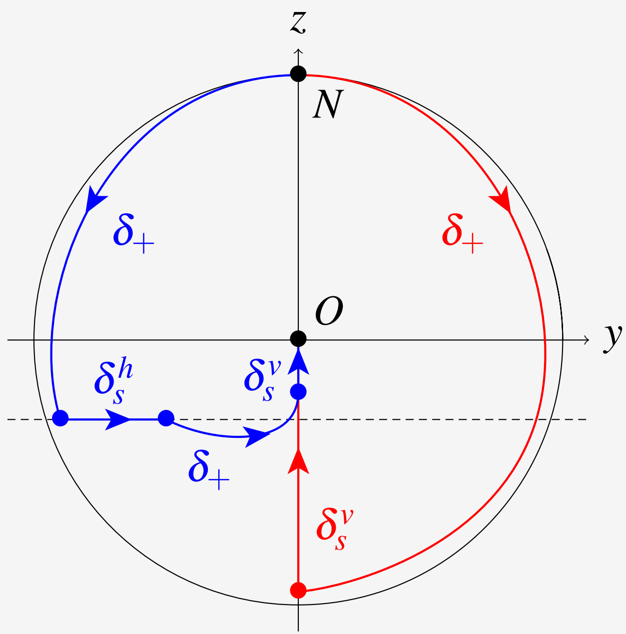
$\Longrightarrow$ $u_s(\boldsymbol{q}, \boldsymbol{p})$ is defined for $(q,p) \in \Sigma_2 : H_G = \{H_G, H_F\} = 0 \setminus \{\{H_G, H_F\}, H_G\} = 0$.

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

Time minimal synthesis for 1 spin (Bonnard et al.) 2012



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: $\dot{q}_i = F_0^i(q_i) + u_1 F_1^i(q_i) + u_2 F_2^i(q_i), \quad i = 1,2$ 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 $w = (q,p) \notin \Sigma = \{w, H_1 = H_2 = 0\}$:

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

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

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

Stratification of the surface $\Sigma = \{w = (q,p), H_1 = H_2 = 0\}$.

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

- If $\boldsymbol{w = (q,p) \in \Sigma_1 = \Sigma \setminus \{H_1, H_2\} = 0}$, 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 $\boldsymbol{w \in \Sigma_2 : H_1 = H_2 = \{H_1, H_2\} = 0 \setminus \det B = 0}$.

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.*

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

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 $u_2 = 0$ $\Longrightarrow \det B = 0$ 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

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

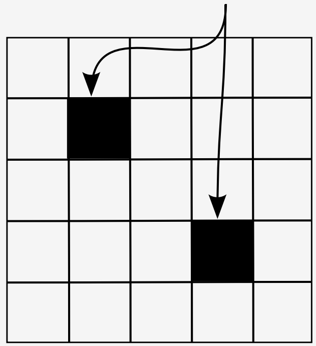
with singular control

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

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.

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



Additionnal constraint: $H = 0$ (t_f free).
Singular control in $H_0 = H_1 = \{H_1, H_0\} = \det B = 0$:

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

$D = \det(F_0, F_1, [F_1, F_0], [[F_1, F_0], F_1])$, $D' = \det(F_0, F_1, [F_1, F_0], [[F_1, F_0], F_0])$.
$\Longrightarrow$ analysis of the flow of $F_0 - D'/D\,F_1$ i.e. of

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

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

Theorem 6. *For $\varepsilon \neq 1$, the equilibirum 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 $(\varepsilon - 1) z_1 y_2 + z_2 y_1 = 0$.*

Algebraic analysis of these components $\Longrightarrow$ computations of equilibirum points.

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