Contrast imaging problem by saturation in nuclear magnetic resonance

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The experiment

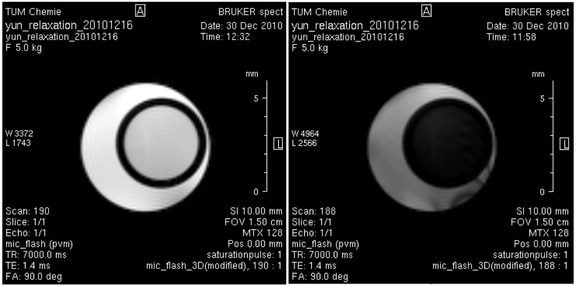


Figure : Experimental results: the samples are placed in two separate test tubes of diameter 5mm and 8mm, and the smaller test tube is placed inside the larger. The inner test tube is filled with deoxygenated blood; the outer tube is filled with oxygenated blood. The two samples at equilibrium are shown on the left, where both appear as white; and the result after the optimal control is applied is shown on the right, where the inner sample appears black, corresponding to the saturation of the first spin, and magnitude of the other sample represents the remaining magnetization.

- M Lapert, Y Zhang, M A Janich, S J Glaser, and D Sugny, *Exploring the Physical Limits of Saturation Contrast in Magnetic Resonance Imaging*, Scientific Reports **2** (2012).
- B. Bonnard, O. Cots, S. J. Glaser, M. Lapert, D. Sugny, and Yun Zhang,*Geometric optimal control of the contrast imaging problem in nuclear magnetic resonance*, IEEE Trans. Automat. Control **57** (2012), no. 8, 1957–1969.

The Bloch equation and the saturation problem

Normalized magnetization vector of a spin 1/2 particle
$M = (x, y, z)$
System

$$\frac{dx}{dt} = -\Gamma x + u_2 z$$
$$\frac{dy}{dt} = -\Gamma y - u_1 z$$
$$\frac{dz}{dt} = \gamma(1 - z) + u_1 y - u_2 x,$$

- γ, Γ: parameters associated to the particle, and $2\Gamma \geq \gamma$
- $N = (0, 0, 1)$: equilibrium point
- Control is a RF magnetic field, $u = (u_1, u_2)$, $|u| \leq 2\pi$
- $M \in B(0, 1)$, the Bloch ball
- $|M|$: "color" between 0 and 1

Saturation problem in minimum time

Set M from the north pole to zero in minimum time

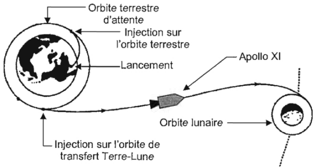
Computation of the optimal solution

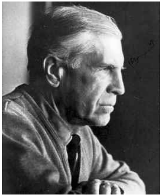
- Parameter $2\Gamma \geq 3\gamma$
- By symmetry of revolution one can restrict to 2D system $\dot{q} = F + uG$, $|u| \leq 2\pi$

$$\begin{cases} \dot{y} = -\Gamma y - uz \\ \dot{z} = \gamma(1 - z) + uy \end{cases}$$

- Simple system but complicated problem

Pontryagin Maximum Principle





Use the Pontryagin Maximum Principle (1956)

$$\text{Lift } (q,u) \to (q,p,u), \quad H = \langle p, \dot{q} \rangle = \langle p, F + uG \rangle$$

Necessary optimality condition for q^*, u^*

$$\begin{cases} \dot{q}^* = \frac{\partial H}{\partial p}(q^*, p^*, u^*) \\ \dot{p}^* = -\frac{\partial H}{\partial q}(q^*, p^*, u^*) \\ H(q^*(t), p^*(t), u^*(t)) = \max_{|v| \leq 2\pi} H(q^*(t), p^*(t), v) \end{cases}$$

Optimal solution

Two types of arcs forming an optimal solution

- $u^*(t) = 2\pi \operatorname{sgn}\langle p^*(t), G^*(q^*(t))\rangle$, "bang-bang" arcs
- $\langle p^*(t), G^*(q^*(t))\rangle = 0$, "singular" arcs

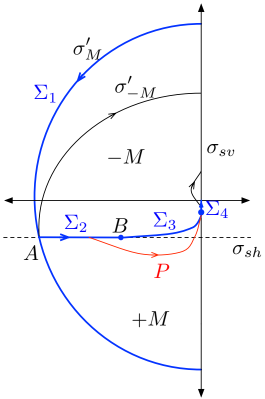
Computation: two singular arcs, one horizontal and one vertical derive $\langle p^*(t), G^*(q^*(t))\rangle = 0$:

$$\langle p, [G, F]\rangle = 0$$

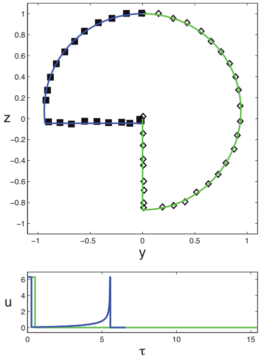
$$\langle p, [[G, F], F]\rangle + u\langle p, [[G, F], G]\rangle = 0$$

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

Optimal solution



(a) Computed optimal solution.



(b) Experimental result. Usual inversion sequence in green, computed sequence in blue.

Contrast problem formulation

Single input case: we fix the control phase and tune only the amplitude u

$$q = (q_1, q_2)$$

$$\begin{cases} \dot{y}_1 = -\Gamma_1 y_1 - u z_1 & \dot{y}_2 = -\Gamma_2 y_2 - u z_2 \\ \dot{z}_1 = \gamma_1 (1 - z_1) + u y_1 & \dot{z}_2 = \gamma_2 (1 - z_2) + u y_2 \end{cases}$$

Contrast problem

- $q_1 \to 0$: Saturation in a fixed transfer time T
- Maximize $|q_2(T)|^2$: final contrast is $|q_2(T)|$

Mayer problem

Mayer problem

- $\frac{dq}{dt} = F(q) + uG(q)$, $|u| \leq 2\pi$
- $\min_{u(\cdot)} c(q(T))$, c : cost
- Terminal condition $g(q(T)) = 0$

Maximum principle

Necessary optimality condition

$$\frac{dq^*}{dt} = \frac{\partial H}{\partial p}, \quad \frac{dp^*}{dt} = -\frac{\partial H}{\partial q}, \quad H(q^*, p^*, u^*) = \max_{|v|\leq 2\pi} H(q^*, p^*, v)$$

Boundary condition

- $q^*(0)$ fixed
- $g(q^*(T)) = 0$
- $p^*(T) = p_0^* \frac{\partial c}{\partial q}(q^*(T)) + \sum_i \sigma_i \frac{\partial g_i}{\partial q_i}(q^*(T))$, $p_0^* \leq 0$ (transversality condition)

Application

As in the saturation problem, but much more complicated.

Two types of arcs

- $u^*(t) = 2\pi \,\mathrm{sgn}\langle p^*(t), G^*(q^*(t))\rangle$, "bang-bang" arcs
- $\langle p^*(t), G^*(q^*(t))\rangle = 0$, "singular" arcs

Complexity: for singular arcs

$$\begin{cases} \langle p, G\rangle = \langle p, [G, F]\rangle = 0 : \Sigma' \\ \langle p, [[G, F], F]\rangle + u_s\langle p, [[G, F], G]\rangle = 0 \end{cases}$$

$$H_s = \langle p, F + u_s G\rangle$$

H_s is a Hamiltonian vector field in dimension 4 with two constraints, $(q, p) \in \Sigma'$.

Analysis of the solution

The maximum principle allows the computation of an optimal candidate using a SHOOTING METHOD

Shooting method

- Compute $p^*(0)$ at the initial time such that (q^*, p^*) is a solution of the maximum principle
- Problem is nonlinear and $p^*(0)$ is not unique
- An initial guess about $p^*(0)$ has to be known to compute the solution using a Newton method. To have such a guess and to determine a priori the structure BSBSBS of the solution we use the Hampath code (O. Cots, 2012).

Numerical continuation method

Regularize Mayer problem into Bolza problem:

$$\min_{u(\cdot)} c(q^*(T)) + (1-\lambda)\int_0^T |u(t)|^{2-\lambda} dt, \quad \lambda \in [0,1]$$

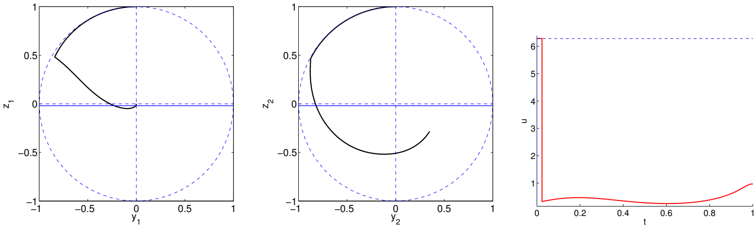
λ : homotopy parameter

Problem "smoothens" $\rightarrow$ Newton method to determine the structure of the solution. Once the structure BSBS is known, compute the solution accurately using a multiple shooting method.

B. Bonnard and O. Cots, *Geometric numerical methods and results in the control imaging problem in nuclear magnetic resonance*, Mathematical Models and Methods in Applied Sciences, to appear.

O. Cots, *Contrôle optimal géométrique : méthodes homotopiques et applications*, Ph.D. thesis, Univ. de Bourgogne, 2012.

Some numerical results



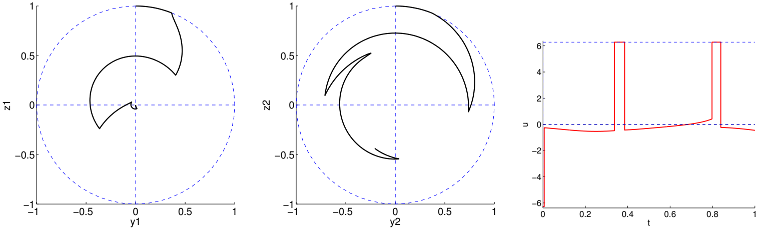
(c) First spin particle, deoxygenated blood

(d) Second spin particle, oxygenated blood

(e) Control, u

Figure : Locally optimal $\sigma_+\sigma_s$ control with contrast 0.449 at time $T = 1.1 \times T_{\min}$ for parameters of deoxygenated and oxygenated blood.

Some numerical results



(a) First spin particle, deoxygenated blood (b) Second spin particle, oxygenated blood (c) Control, u

Figure : A $\sigma_{-}\sigma_{s}\sigma_{+}\sigma_{s}\sigma_{+}\sigma_{s}$ extremal control with contrast 0.484 at time $T = 1.5 \times T_{\min}$ for parameters of deoxygenated and oxygenated blood.

Some numerical results

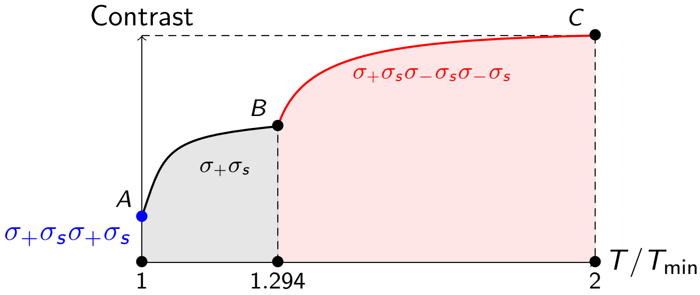


Figure : Synthesis of locally optimal solutions for deoxygenated and oxygenated blood. The solution at A is the time-minimal solution. The path from A to B is the path of zeroes corresponding to the $\sigma_+\sigma_s$ extremal, and the path from B to C is the path of zeroes corresponding to the extremal of structure $\sigma_+\sigma_s\sigma_-\sigma_s\sigma_-\sigma_s$. The two branches cross with the same cost at B, at which point the policy changes from $\sigma_+\sigma_s$ to $\sigma_+\sigma_s\sigma_-\sigma_s\sigma_-\sigma_s$.

Matching computed and experimental results

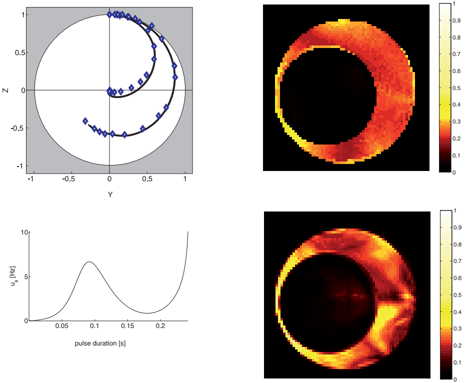


Figure : Computed bang-singular arc in the blood case with experimental result.

Numerical comparison

Direct method (Bocop): Discretization of the optimal control problem

$$
\begin{array}{lcl}
t \in [0, t_f] & \rightarrow & \{t_0 = 0, \ldots, t_N = t_f\} \\
q(\cdot), u(\cdot) & \rightarrow & X = \{q_0, \ldots, q_N, u_0, \ldots, u_{N-1}, t_f\} \\
\hline
\textit{Criterion} & \rightarrow & \min \ c(q_N) \\
\textit{Dynamics} & \rightarrow & (ex : Euler) \ q_{i+i} = q_i + hf(q_i, u_i) \\
\textit{Adm. Cont.} & \rightarrow & -1 \le u_i \le 1 \\
\textit{Bnd. Cond.} & \rightarrow & \Phi(q_0, q_N) = 0
\end{array}
$$

Finite non linear optimization problem:

$$
(NLP) \begin{cases} \min \ F(X) = c(q_N) \\ LB \le C(X) \le UB \end{cases}
$$

LMI (Linear Matrices Inequalities) technics:

In the contrast problem there are many local minima which leads to a very complicated problem: LMI estimates the global optimum.

Direct method

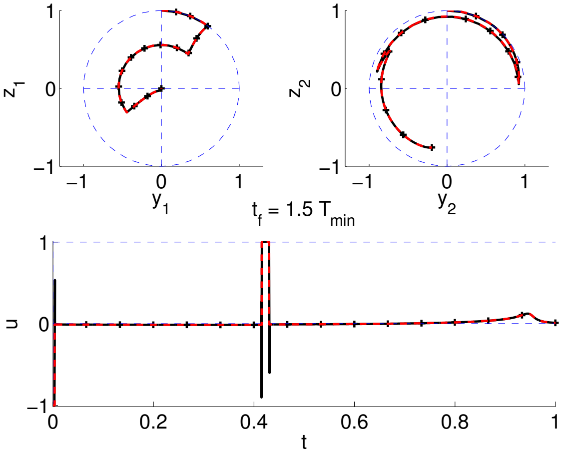


Figure : Cerebrospinal fluid and water case. **Bocop** vs Hampath.

LMI technique

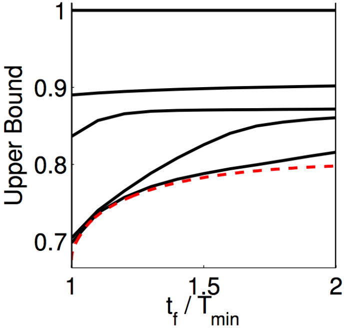


Figure : Cerebrospinal fluid and water case. **LMI** vs Hampath.

B. Bonnard, M. Claeys, O. Cots & P. Martinon,
Complementarities of indirect, direct and moment methods in the contrast imaging problem in NMR,
submitted for 52-nd IEEE Conference on Control Decis., Florence, Italy, (2013).

Experimental problems

We compute the ideal contrast but in practice the different spin particles forming the image are affected by homogeneity of the applied magnetic fields, and the optimal control must be modified to present a more homogeneous result.

M Lapert, Y Zhang, M A Janich, S J Glaser, and D Sugny,
Exploring the Physical Limits of Saturation Contrast in Magnetic Resonance Imaging,
Scientific Reports **2** (2012).

Theoretical problem

- A large amount of work has to be done to understand the controlled Bloch equation
- Role of the relaxation parameters $\rightarrow$ feedback classification
- Dynamical properties of the singular flow