Contrast imaging problem by saturation in nuclear magnetic resonance

Bernard Bonnard

Toronto
november 2014

The experiment

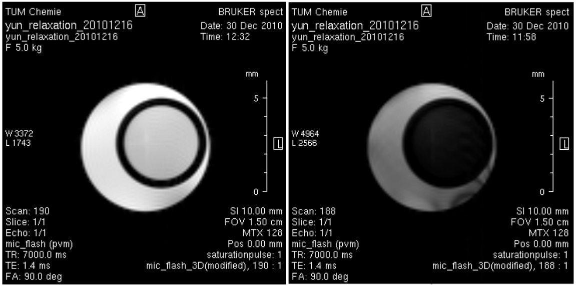


Figure: Experimental results: the samples are placed in two separate test tubes of diameter 5mm and 8mm, and the smaller test tube is placed inside the larger. The inner test tube is filled with deoxygenated blood; the outer tube is filled with oxygenated blood. The two samples at equilibrium are shown 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

Lift $(q, u) \to (q, p, u)$

Use the Pontryagin Maximum Principle (1956)

$$H = \langle p, \dot{q} \rangle = \langle p, F + uG \rangle$$

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

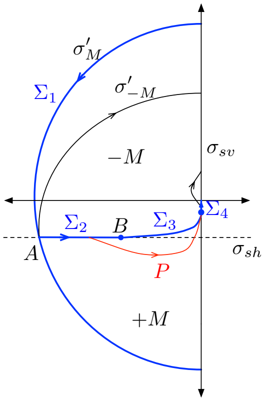
- $u^*(t) = 2\pi \operatorname{sgn}\langle p^*(t), G^*(q^*(t))\rangle$, "bang-bang" arcs
- $\langle p^*(t), G^*(q^*(t))\rangle = 0$, "singular" arcs

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

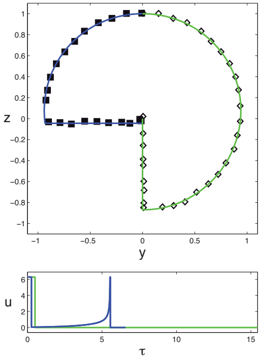
$$\langle p, [G, F]\rangle = 0$$

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

Optimal solution



(a) Computed optimal solution.



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

Contrast problem formulation

$$q = (q_1, q_2)$$

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

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

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

Boundary condition

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

Application

As in the saturation problem, but much more complicated.

Two types of arcs

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

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:

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

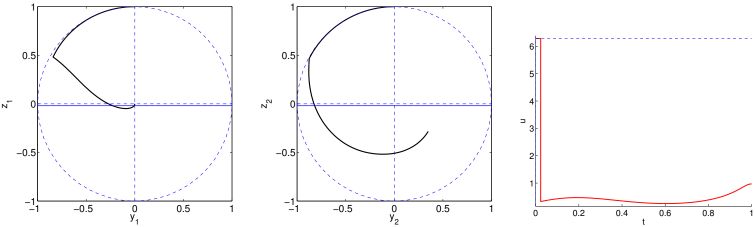
λ : homotopy parameter

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, 2012.

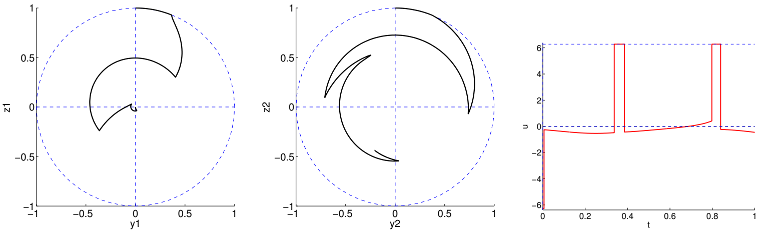
Some numerical results



(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

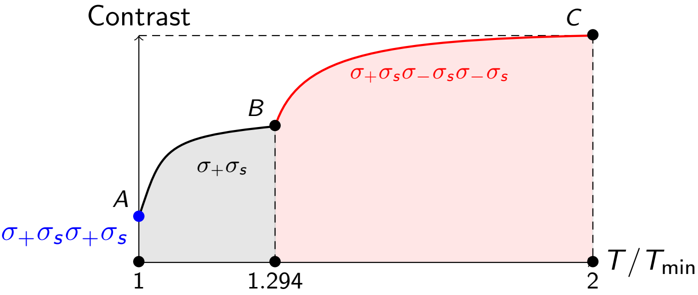


Figure: Synthesis of locally optimal solutions for deoxygenated and oxygenated blood. The solution at A is the time-minimal solution. The path from A to B is the path of zeroes corresponding to the $\sigma_+\sigma_s$ extremal, and the path from B to C is the path of zeroes corresponding to the extremal 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

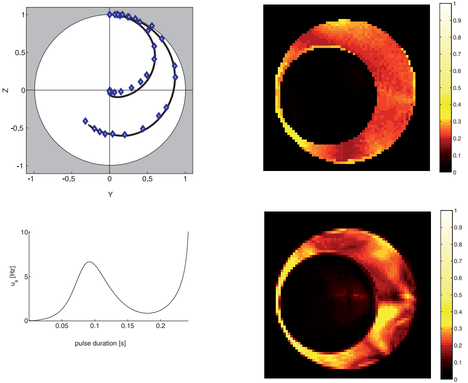


Figure: Computed bang-singular arc in the blood case with experimental result.

Sufficient optimality conditions

The maximum principle is only a necessary optimality condition.

- More conditions have to be found based on the concept of conjugate points.
- Sufficient optimality condition relies on the technique of extremal fields and the Hamilton-Jacobi-Bellman equation.

Remark

In the contrast problem there are many local minima which leads to a very complicated problem.

Works in conplement:

- Direct method BOCOP (Martinon)
- Linear matrix inequality (LMI) techniques (Claeys)

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. WORK IN PROGRESS using BOCOP

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).

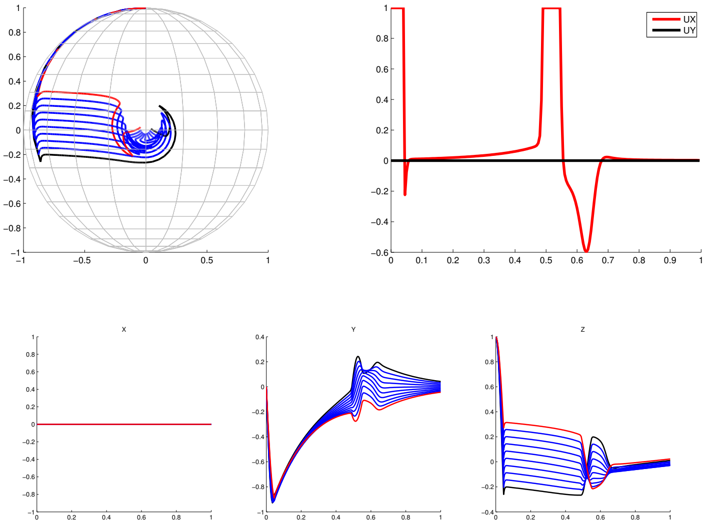
Numerical simulations for saturation with inhomogeneities

Direct transcription method: time discretization
Continuous *OCP* → Finite Dimension *NLP*

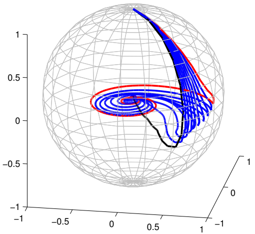
BOCOP: Open source toolbox for optimal control
Dynamics discretized by any Runge-Kutta formula
Nonlinear optimization problem solved by interior point (Ipopt)
Derivatives computed by automatic differentiation (AdolC)
www.bocop.org

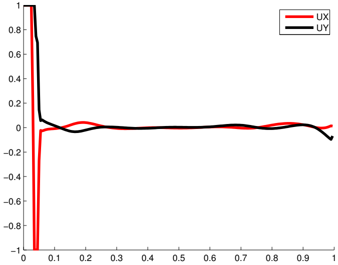
Multi-spin saturation: $Min \ \frac{1}{N}\sum_{i=1}^{N}|q_i(T)|^2$
Final time is fixed as $T = \alpha T_{min}$.
Initial conditions: north pole. Final conditions: none.

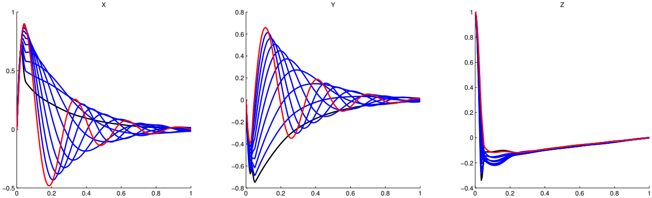
Mono-input, $N = 10$ spins, $B_0 = 0$, $B_1 \in [0, 0.3]$, $T = T_{min}$



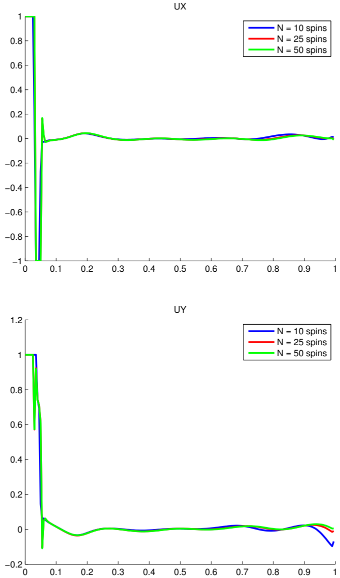
Bi-input, $N = 10$ spins, $B_0 \in [0, 0.5]$, $B_1 \in [0, 0.3]$, $T = T_{min}$

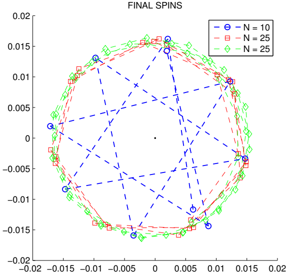






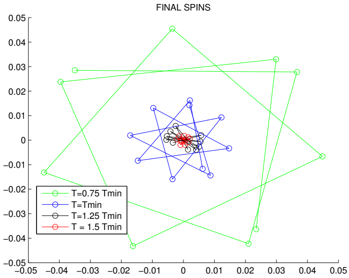
Comparison for $N = 10, 25, 50$ spins

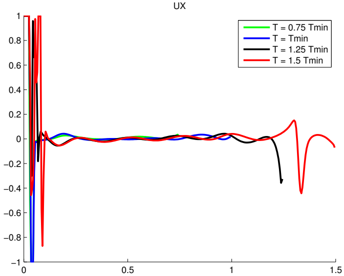


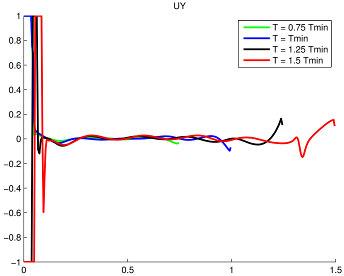


Increasing final time T

T/T_{min}	$\frac{1}{N}\sum_{i=1}^{N}\lvert q_i(T)\rvert^2$
0.75	$2.09\ 10^{-3}$
1	$2.52\ 10^{-4}$
1.25	$3.01\ 10^{-5}$
1.5	$3.36\ 10^{-6}$







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
- Final results, work in progress

Analysis of the singular flow using algebraic-geometric techniques

B. Bonnard, M. Chyba, A. Jacquemard and J. Marriott, *Algebraic geometric classification of the singular flow in the contrast imaging problem in nuclear magnetic resonance*, Mathematical Control and Related Fields, V3, N4, (2013).

- System $\dot{q} = F(q) + u\, G(q), \quad |u| \leq 2\pi \quad q \in \mathbb{R}^4$
- Singular control

$$D = \det(F, G, [G, F], [[G, F], G])$$
$$D' = \det(F, G, [G, F], [[G, F], F])$$

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

$$u_s = -\frac{\langle p, [[G, F], F](q) \rangle}{\langle p, [[G, F], G](q) \rangle}$$

Analysis of the singular flow using algebraic-geometric techniques

- The surface
  $D : \langle p, [[G, F], G](q)\rangle = \langle p, G\rangle = \langle p, [G, F](q)\rangle = 0$
  corresponds to points where $|u_s| \to +\infty$ $\boxed{\text{switching}}$
- Except if $\langle p, [[G, F], F](q)\rangle = 0$ which corresponds to $D = D' = 0$.

Algebraic problem

Compute exactly (with rational coefficients) $\{D = 0\}$, $\{D = 0\} \cap \{D' = 0\}$.

- Reduction : we restrict to the level set $H = 0$ (additional Eq. $\langle p, F \rangle = 0$).
  Hence $\{D = 0\}$ is a dim 3 algebraic variety in $\mathbb{R}^4$,
  $\{D = 0\} \cap \{D' = 0\}$ is a dim 2 algebraic variety in $\mathbb{R}^4$.
- These algebraic varieties depend upon the physical parameters of the chemical species.

Computation and description

- Case | Deoxygenated blood - Oxygenated blood |
- Gröbner basis for $\{D = 0, \nabla D = 0\}$ leads to a direct resolution of a dim 0 algebraic variety.
- We just restrict to roots in $|q| \leq 1$.

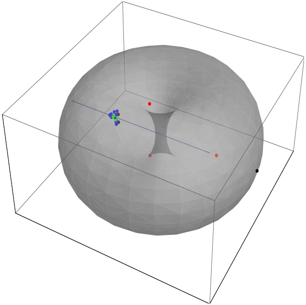


Figure: Complex singularities of $D = 0$

Computation and description

- Analysis of the set $\{D = 0\} \cap \{D' = 0\}$:
  Computation of a Gröbner basis, and then factorization of some of its polynomials, One gets an algebraic description of the two dim 2 components ξ_1, ξ_2, intersecting the Bloch ball. Two coordinates variables are explicitly expressed in terms of rational fractions involving the two others.
- formulæ

$$\xi_1 = \begin{cases} y_1 = \frac{2}{5}\frac{r_1(y_2,z_2)}{p_1(y_2,z_2)} \\ z_1 = \frac{r_2(y_2,z_2)}{p_1(y_2,z_2)} \end{cases}$$

and

$$\xi_2 = \begin{cases} y_1 = \frac{12(34z_2+37)\left(1940y_2^2-219z_2^2-264z_2\right)y_2}{p_2(y_2,z_2)} \\ z_1 = \frac{5\left(51z_2^2-340y_2^2+60z_2\right)\left(1940y_2^2-219z_2^2-264z_2\right)}{p_2(y_2,z_2)} \end{cases}$$

with p_1, p_2, r_1, r_2 polynomials.

Computation of the non-transversal intersection

- Analysis of the points Ξ where $\{D = 0\}$ and $\{D' = 0\}$ are not transversal.
  Computation of sets of Gröbner bases, using factorization and elimination of redundant components.
  No direct parameterization, but characterization of the projections on each spin space.

Non-transversal intersection, projections of Ξ

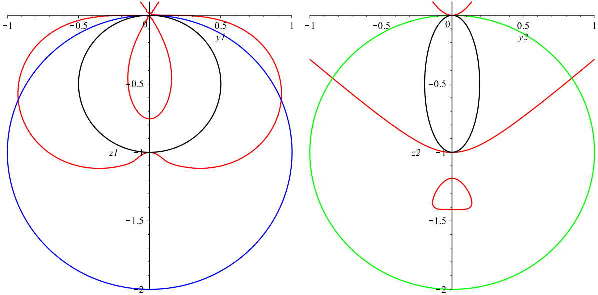


Figure: Projections on (y_1, z_1) (left) and (y_2, z_2) (right) of the singular line Ξ