Geometric and numerical methods in the saturation problem of an ensemble of spin particles.

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Context

- Saturation problem of an ensemble of spin particles in MRI.
  - Mayer optimal control problem
  - Dynamics: Bloch equation
- Geometric tool: Pontryagin Maximum Principle
- Numerical methods
  - Indirect method (*HamPath*): shooting, homotopy…
  - Direct method (*Bocop*): state and control discretizations $\Rightarrow$ NLP problem

Collaborators

[1] with B. Bonnard (Bourgogne Univ.),
S. Glaser, M. Lapert, D. Sugny & Y. Zhang, (Bourgogne & Munich Univ.)
IEEE Trans. Automat. Control (2011).

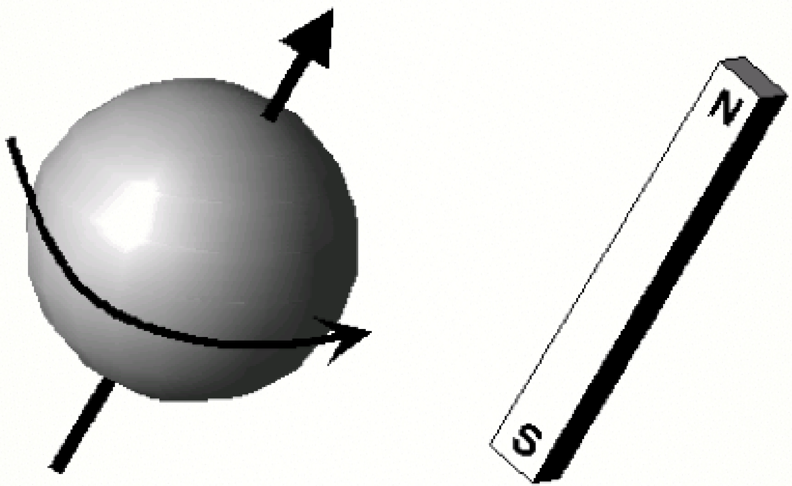
[2] with B. Bonnard,
Math. Models Methods Appl. Sci. (2012).

[3] with B. Bonnard, M. Claeys (LAAS Toulouse) & P. Martinon (INRIA Saclay)
Acta Appl. Math. (2013).

[4] . . .

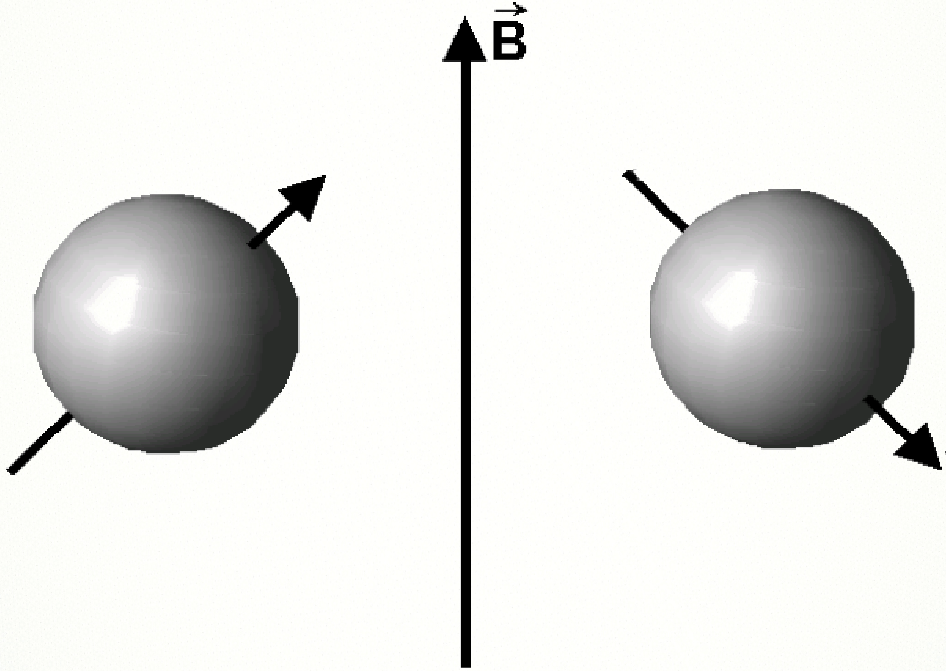
Magnetic moment

Particles of spin-1/2 (proton, neutron, electron…) have magnetic moment.

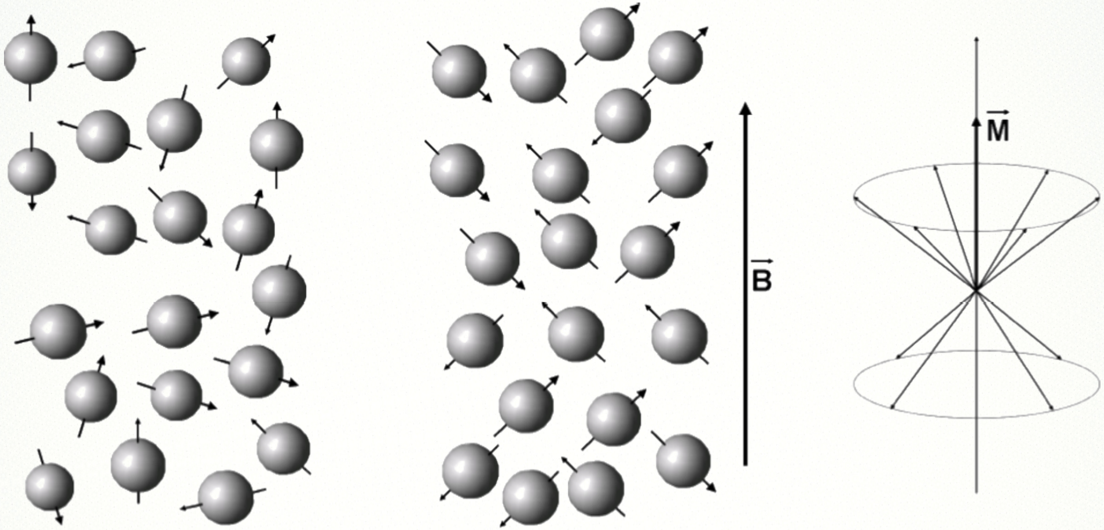


Orientation of the magnetic moment

There are two possible orientations for a spin-1/2 held in a stationary magnetic field $\vec{B}$.



Magnetization vector



(a) (b) (c)

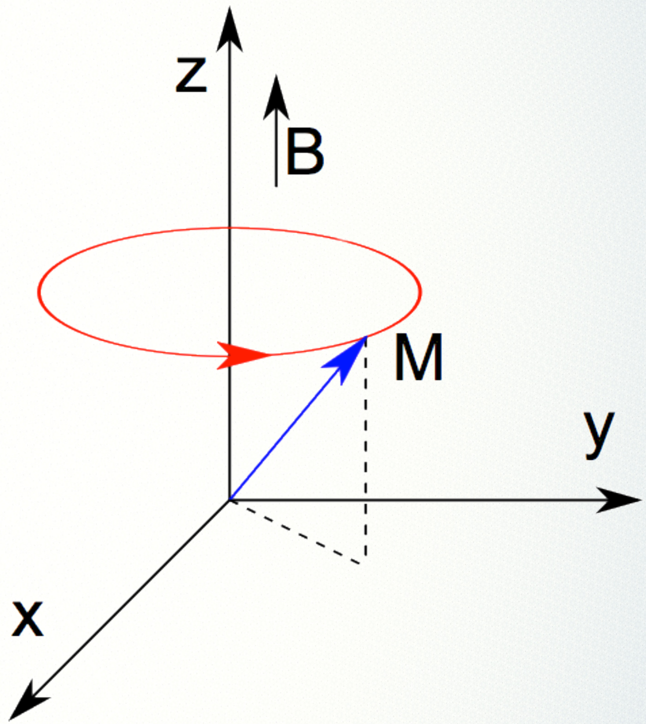
(c) The magnetization vector $\vec{M} = (M_x, M_y, M_z)$ is the sum of the magnetic moments.

$\vec{M}$ is non zero and pointing in the same direction as $\vec{B}$.

Bloch equation.

$$\frac{\mathrm{d}M(t)}{\mathrm{d}t} = \gamma B(t) \wedge M(t),$$

with γ the gyromagnetic ratio.



- Precession around B, with frequency:

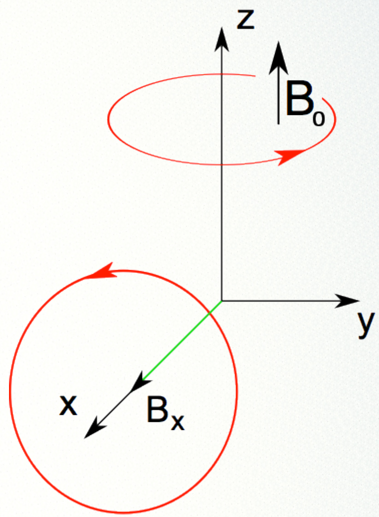
$$\omega = \frac{\gamma}{2\pi} |B|.$$

- Do not change the norm or the direction of M.

Two magnetic fields.

Intense stationary field: $B_0 = (0, \quad 0, \quad B_z)$

Control RF-field: $B_1(t) = (B_x(t), B_y(t), 0)$



✠ $M(t)$ lives on the sphere with radius $M_0 = M(0)$.

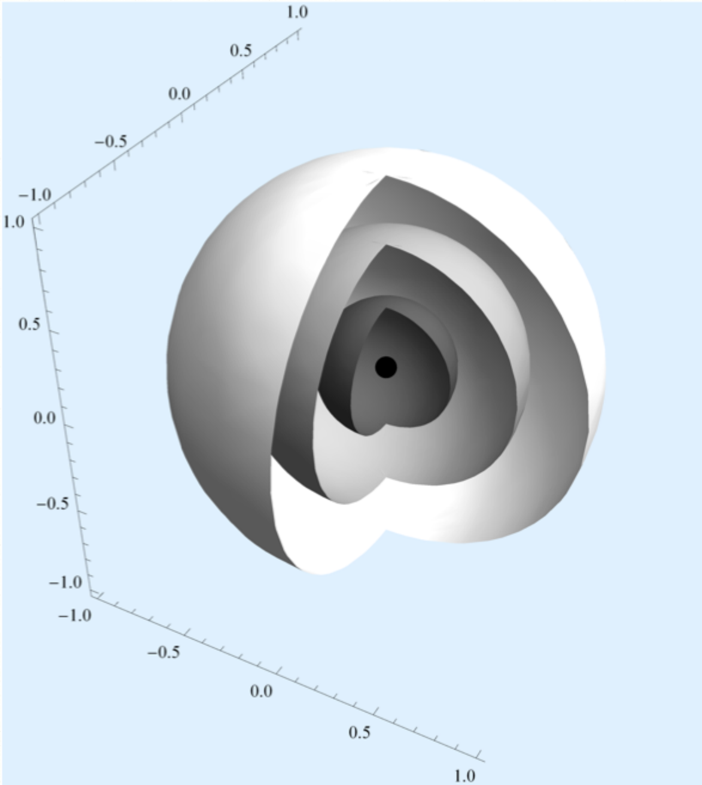
Two relaxation effects. longitudinal (T_1) and transversal (T_2)

$$\dot{M} = R(M, T_1, T_2) + \gamma B \wedge M$$

✠ $M(t)$ lives in the Bloch ball: $|M(t)| \leq M_0$.

Medical Imaging

Medical imaging. The norm of the magnetization vector corresponds to gray scale.



Normalized Dissipative Bloch Equation

Normalized dissipative Bloch equation.

$$\begin{aligned}\dot{x} &= -\Gamma x + u_2 z\\ \dot{y} &= -\Gamma y - u_1 z\\ \dot{z} &= \gamma(1-z) + u_1 y - u_2 x\end{aligned}$$

- State $q = (x, y, z) = M/M_0 \in B(0,1)$: normalized magnetization vector
- $\gamma = 1/T_1$, $\Gamma = 1/T_2$: parameters of the molecule
- Control $u = (u_1, u_2)$, $|u| \leq 1$: normalized RF-field
- $N = (0, 0, 1)$: equilibrium

Saturation of an ensemble of N spins[a].

$$\begin{cases} c(q(t_f)) & = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} |q_i(t_f)|^2 \longrightarrow \min_{u(\cdot)}, \qquad t_f \text{ fixed} \\ \dot{q} & = F_0(q) + u_1 F_1(q) + u_2 F_2(q), \quad |u| \leq 1 \\ q(0) & = q_0 \end{cases}$$

State $q = (q_1, \cdots, q_N)$,

$$q_i = (x_i, y_i, z_i) \in B(0,1), \qquad i = 1, \ldots, N$$

$$q_i(0) = (0,0,1), \qquad i = 1, \ldots, N$$

[a] J. S Li & N. Khaneja, *Control of inhomogeneous quantum ensembles*, Phys. Rev. A., 2006.

Multisaturation Problem with B_1 Inhomogeneity

Saturation of an ensemble of N spins, with B_1 inhomogeneity.

$$\begin{cases} c(q(t_f)) = \dfrac{1}{N}\displaystyle\sum_{i=1}^{N} |q_i(t_f)|^2 \longrightarrow \min_{u(\cdot)}, & t_f \text{ fixed} \\ \dot{q} = F_0(q) + u_1 F_1(q) + u_2 F_2(q), & |u| \leq 1 \\ q(0) = q_0 \end{cases}$$

Scaling factors: a_i, $i = 1, \ldots, N$

$$F_0(q) = \sum_{i=1,N} -\Gamma x_i \frac{\partial}{\partial x_i} - \Gamma y_i \frac{\partial}{\partial y_i} + \gamma(1 - z_i)\frac{\partial}{\partial z_i}$$

$$F_1(q) = \sum_{i=1,N} a_i \left(-z_i \frac{\partial}{\partial y_i} + y_i \frac{\partial}{\partial z_i}\right)$$

$$F_2(q) = \sum_{i=1,N} a_i \left(z_i \frac{\partial}{\partial x_i} - x_i \frac{\partial}{\partial z_i}\right)$$

Pontryagin Maximum Principle

Hamiltonian. $H(q,p,u) = \langle p, \dot{q} \rangle = H_0 + u_1 H_1 + u_2 H_2, \quad H_i = \langle p, F_i(q) \rangle.$

Necessary condition (PMP). If u is optimal, then $\exists\, p : [0, t_f] \to \mathbb{R}^n$ such as a.e.:

$$\dot{q}(t) = \frac{\partial H}{\partial p}(q(t), p(t), u(t)), \quad \dot{p}(t) = -\frac{\partial H}{\partial q}(q(t), p(t), u(t))$$

and

$$H(q(t), p(t), u(t)) = \max_{|v| \leq 2\pi} H(q(t), p(t), v).$$

We have:

$$\begin{cases} u(t) = \dfrac{(H_1, H_2)}{\sqrt{H_1^2 + H_2^2}} \text{ is bang} & \text{if } \sqrt{H_1^2 + H_2^2} \neq 0 \\ u(t) \text{ is singular} & \text{if } H_1 = H_2 = 0 \end{cases}$$

Key roles of Singular extremals and Single-Input case ($u_2 = 0$)

Hamiltonian. $H(q,p,u) = \langle p, \dot{q} \rangle = H_0 + u_1 H_1 + u_2 H_2, \quad H_i = \langle p, F_i(q) \rangle.$

Singular set. $\Sigma := H_1 = H_2 = 0.$

Differentiating H_1, H_2: $\begin{cases} \dot{H}_1 = \{H, H_1\} = H_{01} - u_2 H_{12} = 0 \\ \dot{H}_2 = \{H, H_2\} = H_{02} + u_1 H_{12} = 0 \end{cases}$

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Definitions. Let F_1, F_2 be two vector fields and $z = (q,p)$.

Lie bracket: $F_{12} = [F_1, F_2](q) = \dfrac{\partial F_1}{\partial q}(q) F_2(q) - \dfrac{\partial F_2}{\partial q}(q) F_1(q)$

Poisson bracket: $H_{12} = \{H_1, H_2\}(z) = \mathrm{d}H_1(\vec{H}_2)(z) = H_{[F_1,F_2]}(z), \quad \vec{H}_2 = \begin{pmatrix} \nabla_p H_2 \\ -\nabla_q H_2 \end{pmatrix}.$

KEY ROLES OF SINGULAR EXTREMALS AND SINGLE-INPUT CASE ($u_2 = 0$)

Stratification of $\Sigma := H_1 = H_2 = 0$.

The singular extremals must satisfy:

$$\begin{cases} H_{01} - u_2 H_{12} = 0 \\ H_{02} + u_1 H_{12} = 0 \end{cases}$$

$\Sigma_1 := \Sigma \setminus H_{12} = 0$

- $u_s = \dfrac{(-H_{02}, H_{01})}{H_{12}}$
- Singular extremals in Σ_1 are either not admissible ($|u| > 1$),

  or saturating ($|u| = 1$)

  or not optimal (Goh condition[a]: $H_{12} = 0$).

[a] B. Bonnard & M. Chyba, *Singular trajectories and their role in control theory*, Springer-Verlag, Berlin, 2003.

KEY ROLES OF SINGULAR EXTREMALS AND SINGLE-INPUT CASE ($u_2 = 0$)

Stratification of $\Sigma := H_1 = H_2 = 0$.

The singular extremals must satisfy:

$$\begin{cases} H_{01} - u_2 H_{12} = 0 \\ H_{02} + u_1 H_{12} = 0 \end{cases}$$

If $H_{12} = 0$ then $H_{01} = H_{02} = 0$. Differentiating H_{01}, H_{02}, we get[a]:

$$A\,u_s + b = 0, \text{ with } A = \begin{bmatrix} H_{011} & H_{012} \\ H_{021} & H_{022} \end{bmatrix} \text{ and } b = \begin{bmatrix} H_{010} \\ H_{020} \end{bmatrix}.$$

$\Sigma_2 := H_1 = H_2 = H_{12} = H_{01} = H_{02} = 0 \setminus \det A = 0$

[a] Y. Chitour, F. Jean & E. Trélat, *Genericity results for singular curves*, J. Differential Geom., 2006.

Key roles of Singular extremals and Single-Input case ($u_2 = 0$)

Stratification of $\Sigma := H_1 = H_2 = 0$.

$\Sigma_3 := H_1 = H_2 = H_{12} = H_{01} = H_{02} = \det A = 0$, with $A = \begin{bmatrix} H_{011} & H_{012} \\ H_{021} & H_{022} \end{bmatrix}$

Imposing $u_2 = 0$, each substate $q_i = (x_i, y_i, z_i)$, $i = 1, \ldots, N$, is restricted to $x_i = 0$.

- The corresponding extremals force the surface $\det A = 0$ to be invariant.
- Remaining relations[a] : $H_1 = H_{01} = H_{010} + u_{1,s}\, H_{011} = 0$.
- Legendre-Clebsch condition: $-\dfrac{\partial}{\partial u}\dfrac{\partial^2}{\partial t^2}\dfrac{\partial H}{\partial u} = H_{011} \leq 0$.

[a] I. Kupka, *Geometric theory of extremals in optimal control problems.*, Trans. Amer. Math. Soc., 1987.

Key roles of Singular extremals and Single-Input case ($u_2 = 0$)

Stratification of $\Sigma := H_1 = H_2 = 0$.

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

- Σ_1 of codimension 2: only saturating singular extremals
- Σ_2 of codimension 5: feedback control for $N = 2$
- Σ_3 of codimension 6: contains single-input case ($u_2 = 0$)

Single-input case.

The singular extremals are defined by:

$$H_1 = H_{01} = H_{010} + u_{1,s} H_{011} = 0.$$

Defining $H_s = H_0 + u_{1,s} H_1$, the singular extremals $z = (q, p)$ are solutions of:

$$\frac{\mathrm{d}z}{\mathrm{d}t} = \overrightarrow{H}_s(z), \quad z \in \Sigma_1' := \{z,\ H_1(z) = H_{01}(z) = 0\}, \quad u_{1,s} = -\frac{H_{010}}{H_{011}}.$$

Single-Input case ($u_2 = 0$): Preliminaries

Single-input case with two spins ($N = 2$).

- The dynamics on $q \in \mathbb{R}^4$ can be reduced to:

$$\frac{\mathrm{d}q}{\mathrm{d}t} = F_0(q) - \frac{H_{010}(q,\lambda)}{H_{011}(q,\lambda)} F_1(q), \quad \text{with } \lambda \text{ a one-dimensional parameter.}$$

- Moreover in the exceptional case ($H_0 = 0$), we have:

$$u_{1,s}^e = -D'(q)/D(q)$$

with

$$D = \det(F_0, F_1, F_{10}, F_{101}), \quad D' = \det(F_0, F_1, F_{10}, F_{100})$$

Single-Input case ($u_2 = 0$): Numerical Results

Saturation of an ensemble of 2 spins in the single-input case.

$$\begin{cases} c(q(t_f)) &= \dfrac{1}{2}\displaystyle\sum_{i=1}^{2} |q_i(t_f)|^2 \longrightarrow \min_{u(\cdot)}, \quad t_f \text{ fixed} \\ \dot{q} &= F_0(q) + u_1 F_1(q), \qquad |u_1| \leq 1 \\ q(0) &= q_0 \end{cases}$$

State $q = (q_1, q_2)$, $q_i = (y_i, z_i)$, $|q_i| \leq 1$ and $q_i(0) = (0, 1)$.

$$F_0(q) = \sum_{i=1}^{2} (-\Gamma y_i) \frac{\partial}{\partial y_i} + (\gamma(1 - z_i)) \frac{\partial}{\partial z_i}, \quad F_1(q) = \sum_{i=1}^{2} a_i \left(-z_i \frac{\partial}{\partial y_i} + y_i \frac{\partial}{\partial z_i} \right),$$

Saturation of an ensemble of 2 spins in the single-input case.

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- Blood case: $(\gamma, \Gamma) = \left(\frac{1}{1.35}, \frac{1}{0.05} \right)$
- $t_f = \lambda T_{\min}$, with $T_{\min} = 6.7981$ and $\lambda \in [1, 2]$.
- $(a_1, a_2) = (1, 1 - \varepsilon)$, with $\varepsilon = 0.3$.
- Numerical methods: Direct (*Bocop*[a]) and Indirect (*HamPath*[b]).

[a] http://bocop.org
[b] http://cots.perso.math.cnrs.fr/hampath

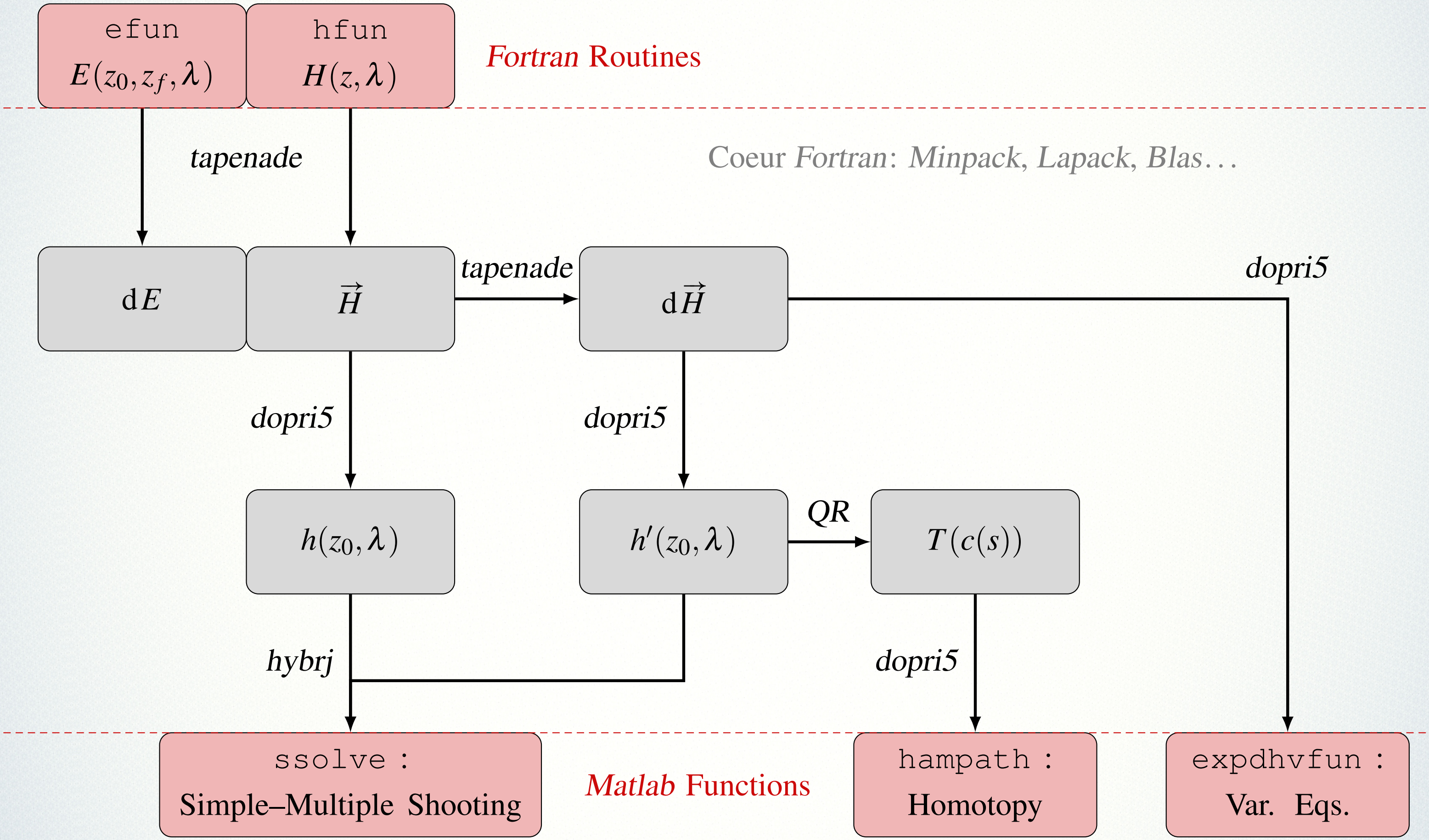
Direct approach. Optimal control problem $(OCP) \Rightarrow$ finite–dimensional optimization problem (NLP), obtained by a discretization in time applied to the state and control variables, as well as the dynamics equation.

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

$$
\Rightarrow (NLP)\left\{\begin{array}{l}
\min\ F(X)=c(q_N) \\
LB \leq C(X) \leq UB
\end{array}\right.
$$

Bocop package. IPOPT solver with MUMPS and ADOL-C for Automatic Differentiation.

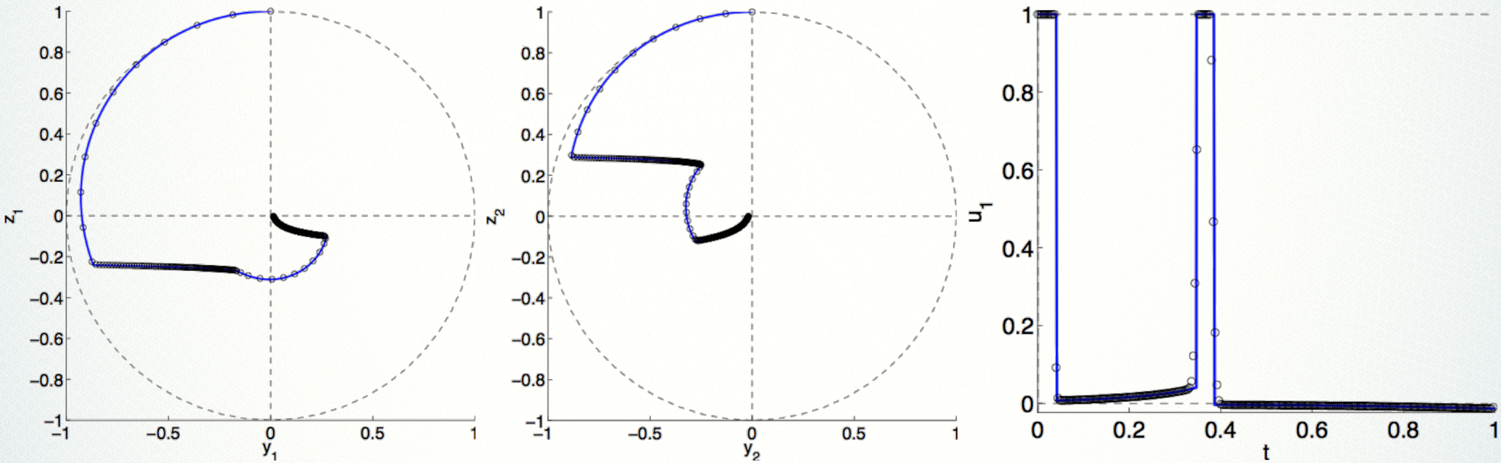
HamPath PACKAGE



Single-Input case ($u_2 = 0$): Numerical Results

Blood case with $N = 2$, $\lambda = 1.1$, $\varepsilon = 0.3$.

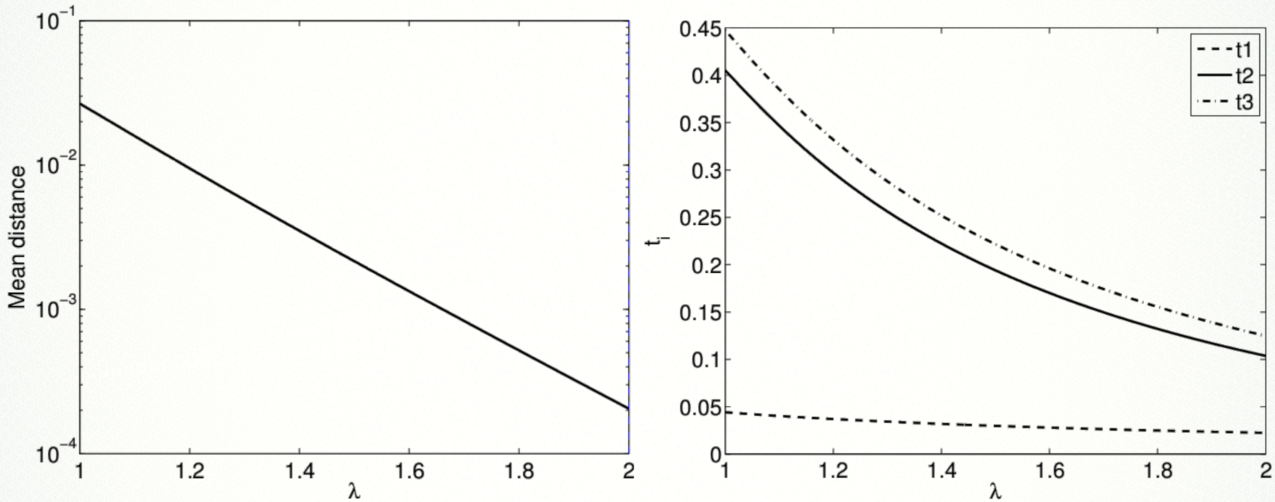
Method	$c(q(t_f))$	initial costate $p(0)$	t_1, t_2, t_3	CPU
Bocop	2.56×10^{-4}	$(2.57, -3.46, -2.96, -4.92) \times 10^{-4}$	$(0.043, 0.338, 0.382)$	0.66s
HamPath	2.56×10^{-4}	$(1.82, -3.85, -3.47, -4.48) \times 10^{-4}$	$(0.040, 0.347, 0.385)$	0.43s



Solution from **direct** (black dots) and indirect (blue line) methods. Control structure is $2BS$.

Single-Input case ($u_2 = 0$): Numerical Results

Homotopy on transfert time (parameter $\lambda = t_f / T_{\min}$).

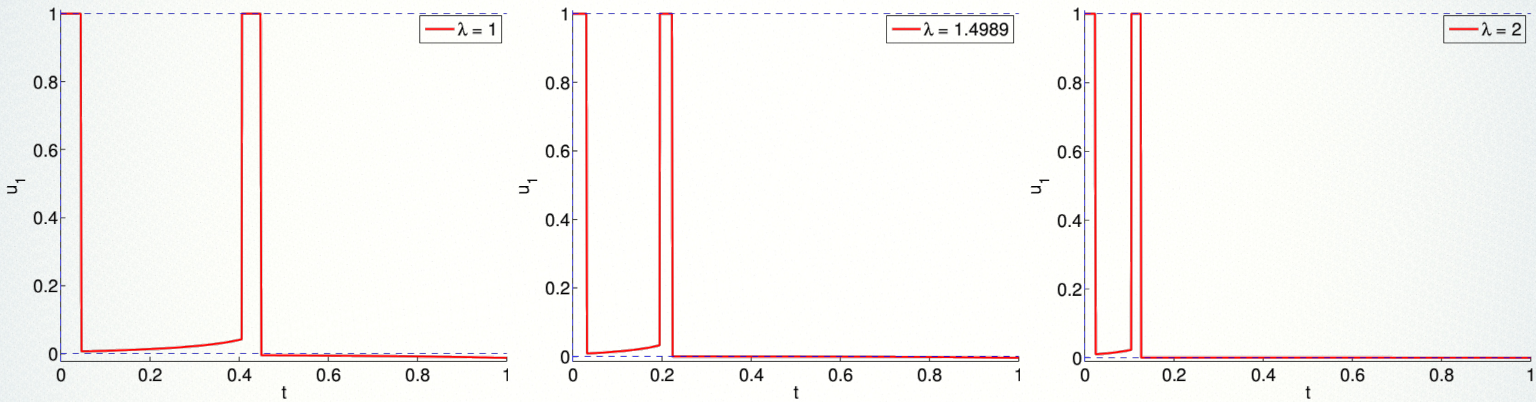


(Left) The mean distance to the origin $\left(\frac{1}{2}\sum_{i=1}^{2} |q_i(t_f)|\right)$ decreases linearly in log scale.

(Right) The switching times indicate a decreasing duration $t_2 - t_1$ for the first singular arc.

Single-Input case ($u_2 = 0$): Numerical Results

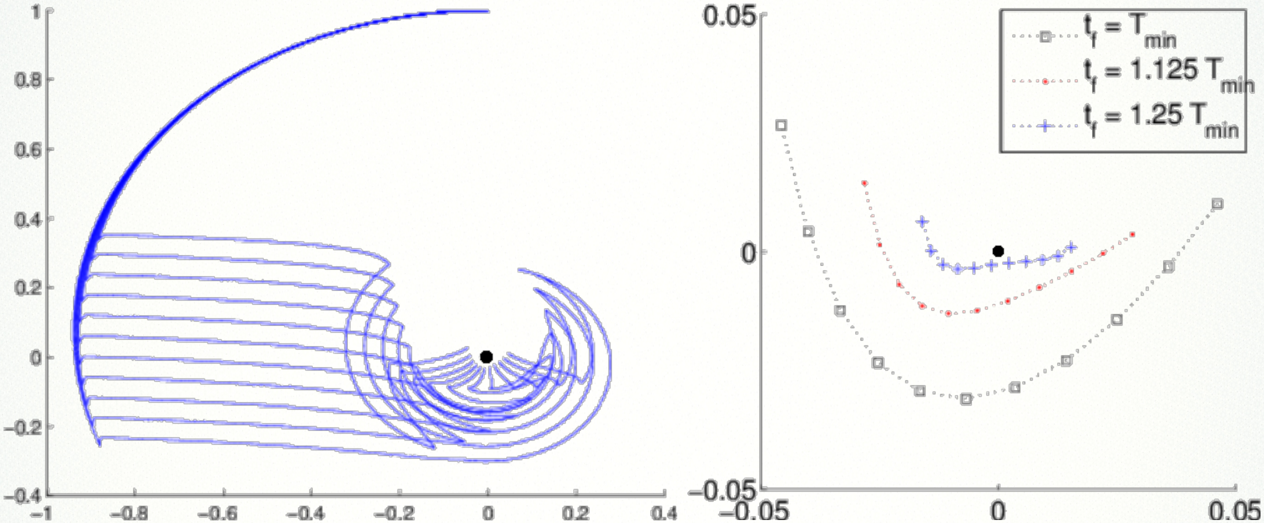
Homotopy on transfert time (parameter $\lambda = t_f / T_{\min}$): controls.



For $\lambda = 1, 1.5$ and 2, the control structure remains $2BS$, with the duration of the first singular arc decreasing for larger λ.

Single-Input case ($u_2 = 0$): Numerical Results

Multisaturation with $N = 11$ spins, with $a_i \in [0.7, 1]$.



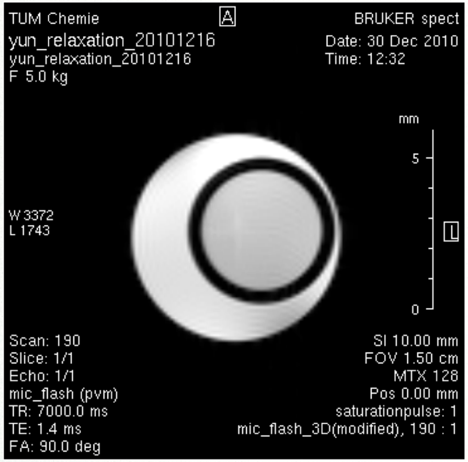
(Left) The trajectory of each spin for $\lambda = 1$ *i.e.* $t_f = T_{\min}$.

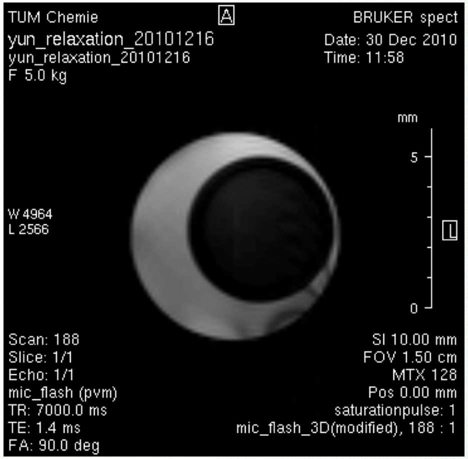
(Right) A closeup on the final positions of all spins for $\lambda = 1, 1.125$ and 1.25.

We observe that the spins tend to spread regularly around the origin, and get closer for larger transfer times.

Multicontrast problem in MRI

We have two different samples (de-oxygenated and oxygenated bloods).





Equilibrium state ⇒ both samples are white.

Optimal control applied ⇒ maximized contrast.

References

[–] N. Khaneja, T. Reiss, C. Kehlet, T. Schulte-Herbrüggen & S. J. Glaser, *Optimal control of coupled spin dynamics: design of NMR pulse sequences by gradient ascent algorithms*, J. of Magn. Reson., **172** (2005), 296–305.

[–] B. Bonnard, O. Cots, S. J. Glaser, M. Lapert, D. Sugny & Y. Zhang, *Geometric optimal control of the contrast imaging problem in nuclear magnetic resonance*, IEEE Trans. Automat. Control, **57** (2012), no 8, 1957 –1969.

[–] B. Bonnard & O. Cots, *Geometric numerical methods and results in the control imaging problem in nuclear magnetic resonance*, Math. Models Methods Appl. Sci., **24** (2014), no. 1, 187–212.

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

[–] B. Bonnard, M. Claeys, O. Cots & P. Martinon, *Geometric and numerical methods in the contrast imaging problem in nuclear magnetic resonance*, Acta Appl. Math., (2013), to appear.