Geometric and numerical methods in optimal control for the time minimal saturation in Magnetic Resonance Imaging

DYNAMICS, CONTROL, and GEOMETRY

In honor of Bronisław Jakubczyk's 70th birthday

12.09.2018 - 15.09.2018 | Banach Center, Warsaw

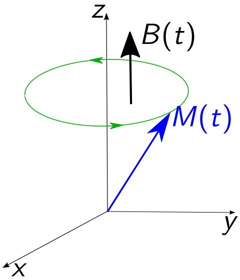
J. Rouot*, B. Bonnard, O. Cots, T. Verron

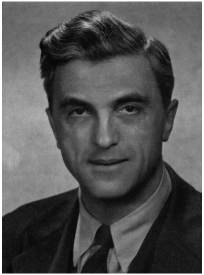
*EPF:Troyes, France, jeremy.rouot@epf.fr

Magnetization vector

• **Bloch equation:** M: magnetization vector of the spin-1/2 particle in a magnetic field $B(t)$.

$$\dot{M}(t) = -\kappa\, M(t) \times B(t)$$





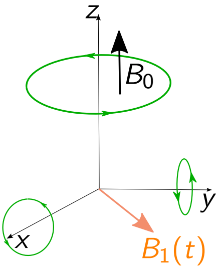
F. Bloch Nobel Prize (1952)

Experimental model in Nuclear Magnetic Resonance

- **Two magnetic fields** : controlled field $B_1(t)$ and
a strong static field B_0

Experimental model in Nuclear Magnetic Resonance

- **Two magnetic fields** : controlled field $B_1(t)$ and a strong static field B_0

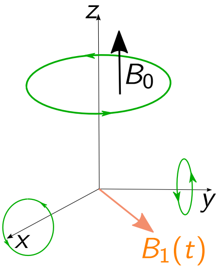


$$\begin{pmatrix} \dot{M}_x \\ \dot{M}_y \\ \dot{M}_z \end{pmatrix} = \begin{pmatrix} -\Gamma M_x \\ -\Gamma M_y \\ -\gamma (M_0 - M_z) \end{pmatrix} + \begin{pmatrix} 0 & -\omega_0 & \omega_y \\ \omega_0 & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{pmatrix} \begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix}$$

- Γ, γ are parameters related to the observed species
- ω_0 is fixed and associated to $\mathbf{B_0}$
- ω_x, ω_y are related to the controlled magnetic field $B_1(t)$

Experimental model in Nuclear Magnetic Resonance

• **Two magnetic fields** : controlled field $B_1(t)$ and a strong static field B_0



$$\begin{pmatrix} \dot{M}_x \\ \dot{M}_y \\ \dot{M}_z \end{pmatrix} = \begin{pmatrix} -\Gamma M_x \\ -\Gamma M_y \\ -\gamma (M_0 - M_z) \end{pmatrix} + \begin{pmatrix} 0 & -\omega_0 & \omega_y \\ \omega_0 & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{pmatrix} \begin{pmatrix} M_x \\ M_y \\ M_z \end{pmatrix}$$

- Γ, γ are parameters related to the observed species
- ω_0 is fixed and associated to $\mathbf{B_0}$
- ω_x, ω_y are related to the controlled magnetic field $B_1(t)$

• $M(t) \in S(O, |M(0)|)$,
$B_1 \equiv 0 \Rightarrow$ relaxation to the stable equilibrium $M = (0, 0, |M(0)|)$.

- Normalized Bloch equation in the *rotating frame* $(\omega_0, (Oz))$

$$\begin{aligned} \dot{x}(t) &= -\Gamma\, x(t) + u_y(t)\, z(t), \\ \dot{y}(t) &= -\Gamma\, y(t) - u_x(t)\, z(t), \\ \dot{z}(t) &= \gamma\,(1 - z(t)) - u_y(t)\, x(t) + u_x(t)\, y(t). \end{aligned}$$

  - $q = (x, y, z) = M/M(0)$ is the normalized magnetization vector,
  - (u_x, u_y) is the control.

- Normalized Bloch equation in the *rotating frame* $(\omega_0, (Oz))$

$$\begin{aligned}
\dot{x}(t) &= -\Gamma\, x(t) + u_y(t)\, z(t), \\
\dot{y}(t) &= -\Gamma\, y(t) - u_x(t)\, z(t), \\
\dot{z}(t) &= \gamma\,(1 - z(t)) - u_y(t)\, x(t) + u_x(t)\, y(t).
\end{aligned}$$

  - $q = (x, y, z) = M/M(0)$ is the normalized magnetization vector,
  - (u_x, u_y) is the control.

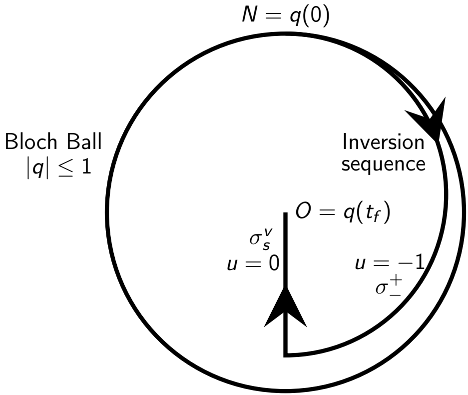
- Symmetry of revolution around (Oz), we set: $u_y = 0$ and we obtain the **planar control system**

$$\begin{aligned}
\dot{y}(t) &= -\Gamma\, y(t) - u(t)\, z(t), \\
\dot{z}(t) &= \gamma\,(1 - z(t)) + u(t)\, y(t),
\end{aligned}$$

and $u = u_x$ is the control satisfying $|u| \leq 1$.

Saturation of a single spin in minimum time

- **Aim**. Steer the North pole $N = (0,1)$ of the Bloch ball $\{|q| \leq 1\}$ to the center O in minimum time.



The inversion sequence $\sigma_-^N \sigma_s^v$ is not optimal in many physical cases

- **Pontryagin Maximum Principle.**
  - Pseudo-Hamiltonian: $H(q,p,u) = p \cdot (F(q) + u\,G(q)) = H_F + u\,H_G$
  - $u(\cdot)$ optimal $\Rightarrow \exists p(\cdot) \in \mathbb{R}^2 \setminus \{0\}$:

$$\dot q = \frac{\partial H}{\partial p}, \quad \dot p = -\frac{\partial H}{\partial q}$$

$$H(q(t),p(t),u(t)) = \max_{|v|\le 1} H(q(t),p(t),v) = cst \ge 0$$

  - Regular and bang-bang controls: $u(t) = \mathrm{sign}(H_G(q(t),p(t)))$, $H_G(q(t),p(t)) \neq 0$
  - Singular trajectories are contained in $\{q,\ \det(G,[F,G])(q) = 0\}$:

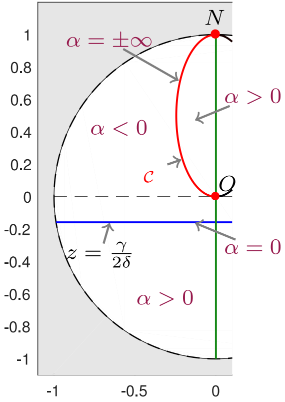
$$z = \gamma/(2\,\delta) = z_s(\gamma,\Gamma),\ \delta = \gamma - \Gamma \quad \text{and} \quad y = 0.$$

Computations:

$$D'(q) + u\, D(q) = 0$$

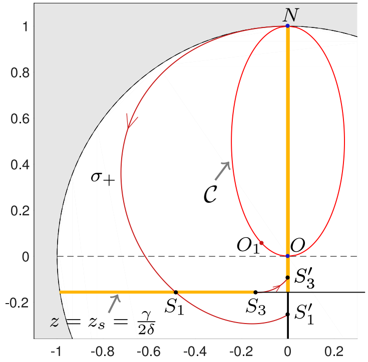
with $D = \det(G, [G, [F, G]])$ and $D' = \det(G, [F, [F, G]])$.
We obtain:

- $u_s = \gamma(2\Gamma - \gamma)/(2\delta y)$ on the horizontal singular line.
- $u_s = 0$ on the vertical singular line



- Symmetry: $u \leftarrow -u$ corresponds to $y \leftarrow -y$
- Collinearity set:
  $\mathcal{C} = \{q \mid \det(F, G)(q) = 0\}$
- Switching function:
  $\Phi(t) = p(t) \cdot G(q(t))$ and outside the set $\mathcal{C}$,
  $\text{sign}(\dot{\Phi}(t)) = \text{sign}(\alpha(q))$, $\alpha(q) \neq 0$
  where $\alpha(q(t)) = \dfrac{\det(G, [F, G])(q)}{\det(G, F)(q)}$.

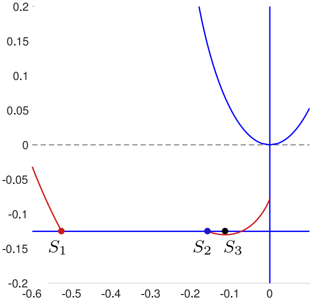
Definition of the points S_1, S_3



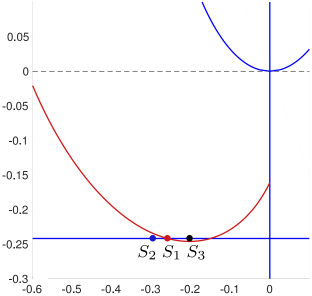
The singular trajectory $q(\cdot)$ is called

- *Hyperbolic* if $p(t) \cdot [G, [F, G]](q(t)) = \frac{\partial}{\partial u} \frac{\mathrm{d}^2}{\mathrm{d}t^2} \frac{\partial H}{\partial u}(q(t), p(t)) > 0$.
- *Elliptic* if $p(t) \cdot [G, [F, G]](q(t)) = \frac{\partial}{\partial u} \frac{\mathrm{d}^2}{\mathrm{d}t^2} \frac{\partial H}{\partial u}(q(t), p(t)) < 0$.

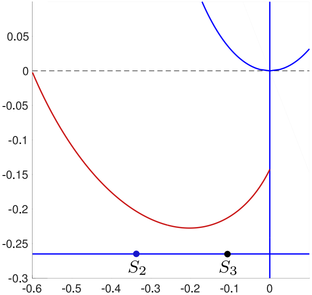
Optimal synthesis depends on the ratio $\frac{\gamma}{\Gamma}$.



Case 1: S_1 exists and $S_2 \in S_1S_3$

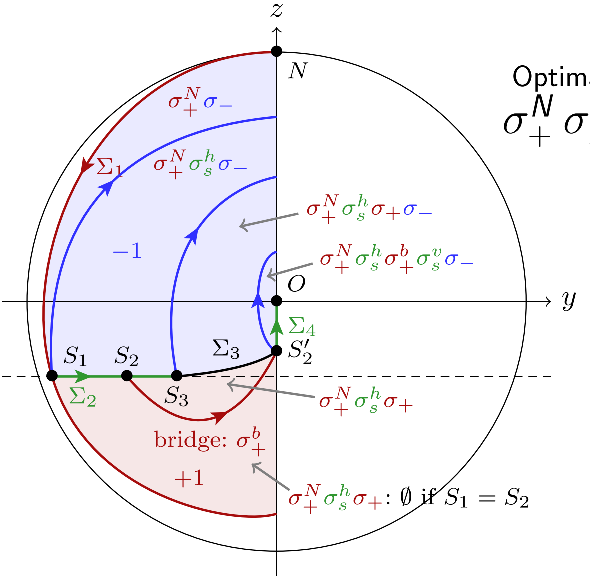


Case 2: S_1 exists and $S_2 \notin S_1S_3$



Case 3: S_1 doesn't exist

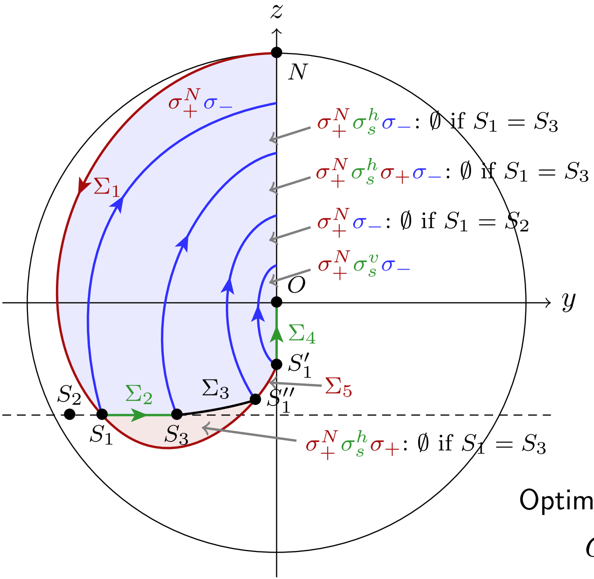
Case 1: S_1 exists and $S_2 \in S_1S_3$



Optimal trajectory from N to O:

$$\sigma_+^N \sigma_s^h \sigma_+^b \sigma_s^v$$

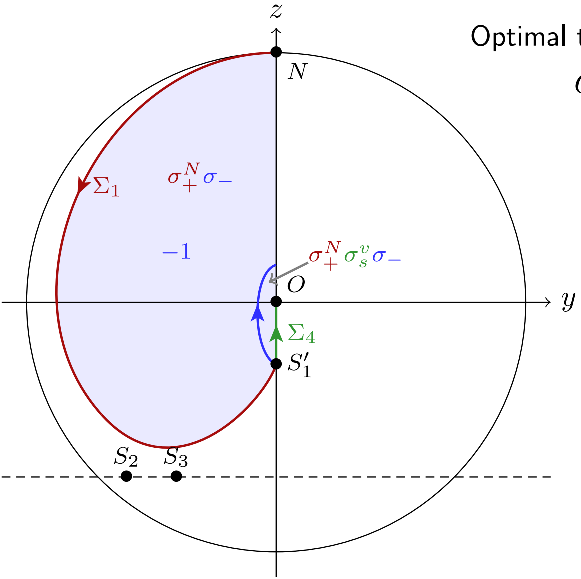
Case 2: S_1 exists and $S_2 \notin S_1S_3$



Optimal trajectory from N to O:

$$\sigma_+^N \sigma_s^v$$

Case 3: S_1 doesn't exists



Optimal trajectory from N to O:

$$\sigma_+^N \sigma_s^v$$

Theorem

The time optimal trajectory for the saturation problem of 1-spin is of the form:

$$\sigma_+^N \quad \underbrace{\sigma_s^h \quad \sigma_+^b}_{\text{empty if } S_2 \le S_1} \quad \sigma_s^v$$

Numerical validations using Moments/LMI techniques

Aim: Provide lower bounds on the global optimal time.

- Numerical times obtain with the `HamPath` software to validate :

Case	Γ	γ	t_f
C_1	9.855×10^{-2}	$3.65\ \times10^{-3}$	42.685
C_2	2.464×10^{-2}	$3.65\ \times10^{-3}$	110.44
C_3	1.642×10^{-2}	2.464×10^{-3}	164.46
C_4	9.855×10^{-2}	9.855×10^{-2}	8.7445

Context

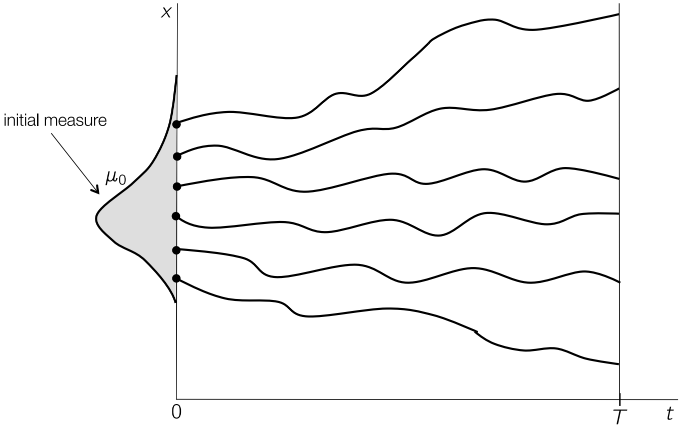
$$t_f = \inf_{u(\cdot)} \; T$$
$$\dot{x}(t) = f(x(t), u(t)),$$
$$x(t) \in X, \quad u(t) \in U, \quad x(0) \in X_0, \quad x(T) \in X_T$$

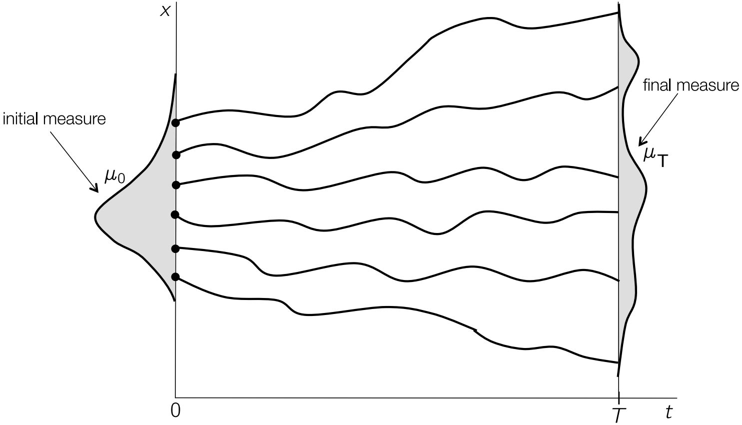
X, U, X_0, X_T are subsets of $\mathbb{R}^n$ which can be written as

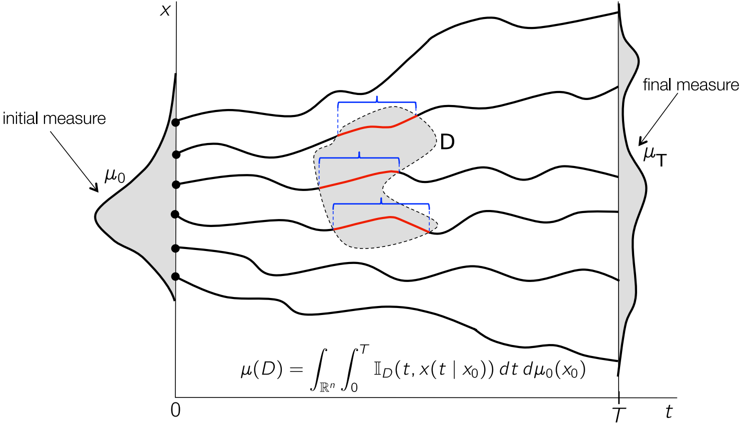
$$X = \{(t,x) : p_k(t,x) \geq 0,\ k = 0, \ldots, n_X\},\ U = \{u : q_k(u) \geq 0,\ k = 0, \ldots, n_U\}$$
$$X_0 = \{x : r_k^0(x) \geq 0,\ k = 0, \ldots, n_0\},\ X_T = \{(t,x) : r_k^T(t,x)0,\ k = 0, \ldots, n_T\}$$

Objective: Compute $\min_{u(\cdot)} T$ when $f, p_k, q_k, r_k^0, r_k^T$ are polynomials and the above sets are compacts.

Result: [J. B. Lasserre, D. Henrion, C. Prieur, E. Trélat, 2008]
Converging monotone nondecreasing sequence of lower bounds of t_f.


x
initial measure
μ_0
0
T
t


x
initial measure
μ_0
final measure
μ_T
0
T
t



$$\int_0^T v(t, x(t))\,\mathrm{d}t = \int_0^T \int_X \int_U v(t, x)\,\mathrm{d}\mu(t, x, u), \quad v \in \mathcal{C}^0([0, T] \times X)$$

Liouville's equation

Linear equation linking the measures μ_0, μ and μ_T.

$$\int_{X_T} v(T,x)\,\mathrm{d}\mu_T(x) - \int_{X_0} v(0,x)\,\mathrm{d}\mu_0(x) = \int_{[0,T]\times Q\times U} \frac{\partial v}{\partial t} + \nabla_x \cdot f(x,u)\,\mathrm{d}\mu(t,x,u)$$

for all test functions $v \in \mathcal{C}^1([0,T] \times X)$.

Optimization over system trajectories

$\Leftrightarrow$

Optimization over measures satisfying Liouville equation.

- **Relaxed controls:** $u(t)$ is replaced for each t by a probability measure $\omega_t(u)$ supported on U.
- **Relaxed problem:**

$$T_R = \min_{\omega} \; T$$

$$s.t. \quad \dot{x}(t) = \int_U f(x(t), u)\, \mathrm{d}\omega_t(u)$$

$$x(0) \in X_0, \quad x(t) \in X, \quad x(T) \in X_T$$

- **Relaxed controls:** $u(t)$ is replaced for each t by a probability measure $\omega_t(u)$ supported on U.
- **Relaxed problem:**

$$T_R = \min_{\omega} \; T$$
$$\text{s.t.} \quad \dot{x}(t) = \int_U f(x(t), u)\,\mathrm{d}\omega_t(u)$$
$$x(0) \in X_0, \quad x(t) \in X, \quad x(T) \in X_T$$

- **Linear Problem on measures:**
$\mathrm{d}\mu(t,x,u) = \mathrm{d}t\,\mathrm{d}\delta_{x(t)}(x)\,\mathrm{d}\omega_t(u) \in \mathcal{M}_+([0,T] \times X \times U)$

$$T_{LP} = \min_{\mu, \mu_T, \mu_0} \int \mathrm{d}\mu_T$$
$$\text{s.t.} \int \Big(\frac{\partial v}{\partial t} + \frac{\partial v}{\partial x} f(x,u) \Big) \mathrm{d}\mu$$
$$= \int v(\cdot, x_T)\mathrm{d}\mu_T - \int v(0, x_0)\mathrm{d}\mu_0, \quad \forall v \in \mathbb{R}[t,x],$$
$$\mu \in \mathcal{M}_+([0,T] \times X \times U), \quad \mu_T \in \mathcal{M}_+(X_T), \quad \mu_T \in \mathcal{M}_+(X_0)$$

Notation: $\alpha = (\alpha_1, \ldots, \alpha_p) \in \mathbb{N}^p,\ z = (z_1, \ldots, z_p) \in \mathbb{R}^p$. We denote by z^α the monomial $z_1^{\alpha_1} \ldots z_p^{\alpha_p}$ and by $\mathbb{N}_d^p$ the set $\{\alpha \in \mathbb{N}^p, |\alpha|_1 = \sum_{i=1}^p \alpha_i \leq d\}$.

Moment of order α for a measure $\nu \in \mathcal{M}_+(Z)$: $y_\alpha^\nu = \int z^\alpha \,\mathrm{d}\nu(z)$.

Riesz linear functional: $l_{y^\nu} : \mathbb{R}[z] \to \mathbb{R}$ s.t. $l_{y^\nu}(z^\alpha) = y_\alpha^\nu$.

Moment Matrix: $M_d(y^\nu)[i,j] = y_{i+j}^\nu,\ \forall i,j \in \mathbb{N}_d^p$.

Notation: $\alpha = (\alpha_1, \ldots, \alpha_p) \in \mathbb{N}^p,\ z = (z_1, \ldots, z_p) \in \mathbb{R}^p$. We denote by z^α the monomial $z_1^{\alpha_1} \ldots z_p^{\alpha_p}$ and by $\mathbb{N}_d^p$ the set $\{\alpha \in \mathbb{N}^p, |\alpha|_1 = \sum_{i=1}^p \alpha_i \leq d\}$.

Moment of order α for a measure $\nu \in \mathcal{M}_+(Z)$: $y_\alpha^\nu = \int z^\alpha \, \mathrm{d}\nu(z)$.

Riesz linear functional: $l_{y^\nu} : \mathbb{R}[z] \to \mathbb{R}$ s.t. $l_{y^\nu}(z^\alpha) = y_\alpha^\nu$.

Moment Matrix: $M_d(y^\nu)[i,j] = y_{i+j}^\nu,\ \forall i,j \in \mathbb{N}_d^p$.

Proposition (Putinar, 1993)

Let $Z = \{z \in \mathbb{R}^p \mid g_k(z) \geq 0,\ k = 1, \ldots, n_Z\}$. The sequence $(y_\alpha)_\alpha$ has a representing measure $\nu \in \mathcal{M}_+(Z)$ if and only if

$$M_d(y) \succeq 0, \quad M_d(g_k\, y) \succeq 0, \quad \forall d \in \mathbb{N}, \forall k = 1, Moment \ldots, n_Z.$$

Moment Semidefinite Programming Problem:

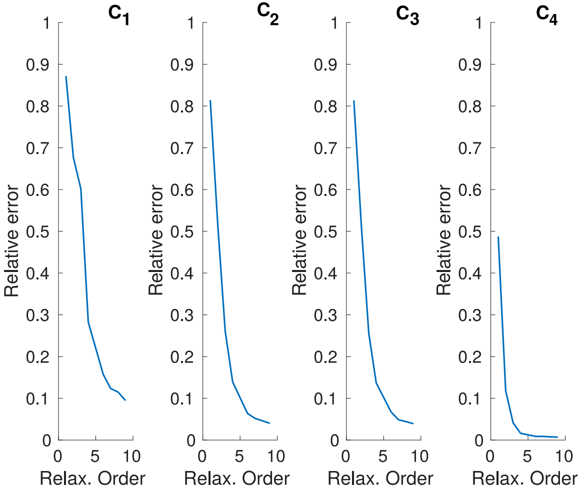
$$
\begin{aligned}
T_{SDP} = \min_{y^{\mu}, y^{\mu_T}} \; & l_{y^{\mu_T}}(1) \\
& l_{y^{\mu}}\left(\frac{\partial v}{\partial t} + \frac{\partial v}{\partial x} f(x,u)\right) = l_{y^{\mu_T}}(v(\cdot, x_T)) - l_{y^{\mu_0}}(v(0,x_0)),\ \forall v \in \mathbb{R}[t,x], \\
& M_d(y^{\mu}) \succeq 0,\ M_d(g_i\, y^{\mu}) \succeq 0,\ \forall i,\ \forall d \in \mathbb{N}, \\
& M_d(y^{\mu_0}) \succeq 0,\ M_d(g_i^0\, y^{\mu_T}) \succeq 0,\ \forall i\ \forall d \in \mathbb{N} \\
& M_d(y^{\mu_T}) \succeq 0,\ M_d(g_i^T\, y^{\mu_T}) \succeq 0,\ \forall i\ \forall d \in \mathbb{N}
\end{aligned}
$$

where g_i, g_i^0 and g_i^T are polynomials defining the sets $[0, T] \times X \times U$, X_0 and X_T respectively.

By truncating the sequences $(y^\mu), (y^{\mu_T})$ up to moments of length r (relaxation order), we have a **hierarchy of Semidefinite Programming Problems** and the lower bounds $T^1_{sdp}, \ldots, T^r_{sdp}, \ldots$ of these problems satisfy:

$$t_f = T_{LP} = T_{SDP} \geq \ldots \geq T^{r+1}_{sdp} \geq T^r_{sdp} \geq \ldots \geq T^1_{sdp}.$$

Numerical results on the saturation problem



Perspectives

- Generalization to an ensemble of pair of spins where Bloch equations are coupled and Inhomogeneities on the control field are taken into account.
- Contrast problem where we have two species to discriminate. Saturation of the first spin while the norm of the second spin is maximized.