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

Jérémy Rouot, Bernard Bonnard, Olivier Cots, Thibaut Verron

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

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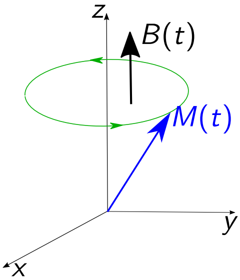
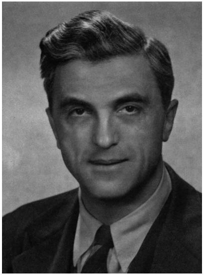
Magnetization vector

• **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
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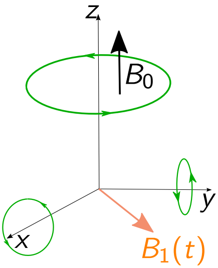

$$\begin{pmatrix} \dot{M}_x \\ \dot{M}_y \\ \dot{M}_z \end{pmatrix} = \begin{pmatrix} -\Gamma\, M_x \\ -\Gamma\, M_y \\ -\gamma\,(M_0 - M_z) \end{pmatrix} + \begin{pmatrix} 0 & -\omega_0 & \omega_y \\ \omega_0 & 0 & -\omega_x \\ -\omega_y & \omega_x & 0 \end{pmatrix} \begin{pmatrix} M_x \\ M_y \\ M_z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

- 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 $B_1(t)$

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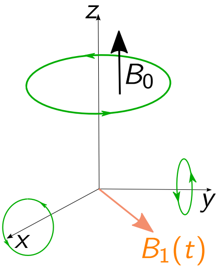

- **Two magnetic fields** : controlled field $B_1(t)$ and a strong static field B_0

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

  - 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* $(\omega_0, (Oz))$

$$
\begin{aligned}
\dot{x}(t) &= -\Gamma\, x(t) + u_y(t)\, z(t), \\
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$$

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

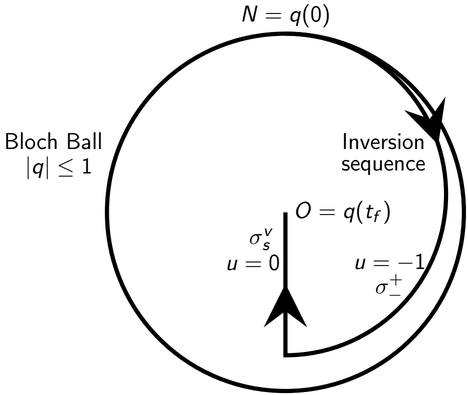
- Symmetry of revolution around (Oz), we set: $u_y = 0$ and we obtain the **planar control system**

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

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

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 $\Rightarrow \exists p(\cdot) \in \mathbb{R}^2 \setminus \{0\}$:

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

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

  - 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 $\{q,\ \det(G, [F, G])(q) = 0\}$:

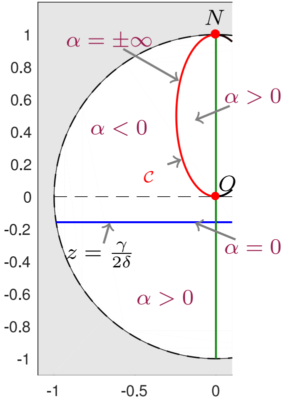
$$z = \gamma/(2\,\delta) = z_s(\gamma, \Gamma),\ \delta = \gamma - \Gamma \quad \text{and} \quad y = 0.$$

Computations:

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

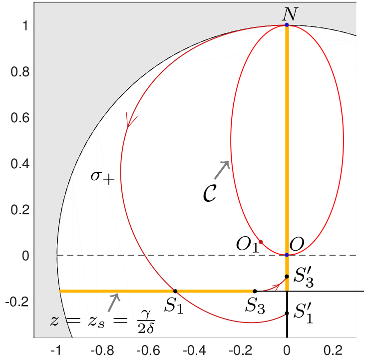
with $D = \det(G, [G, [F, G]])$ and $D' = \det(G, [F, [F, G]])$.
We obtain:

- $u_s = \gamma(2\Gamma - \gamma)/(2\delta y)$ 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 $\mathcal{C}$, $\operatorname{sign}(\dot\Phi(t)) = \operatorname{sign}(\alpha(q))$, $\alpha(q) \neq 0$ where $\alpha(q(t)) = \dfrac{\det(G, [F, G])(q)}{\det(G, F)(q)}$.

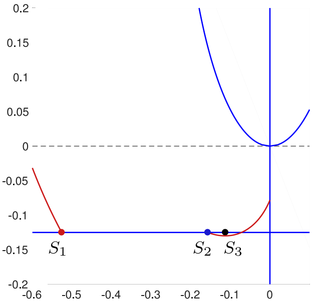
Definition of the points S_1, S_3



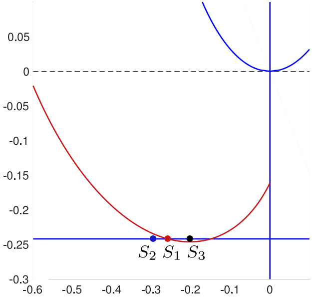
The singular trajectory $q(\cdot)$ is called

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

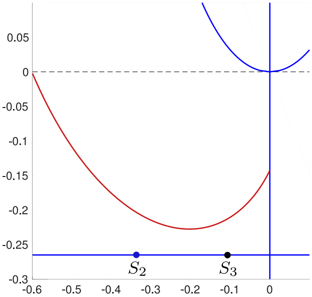
Optimal synthesis depends on the ratio $\frac{\gamma}{\Gamma}$.



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

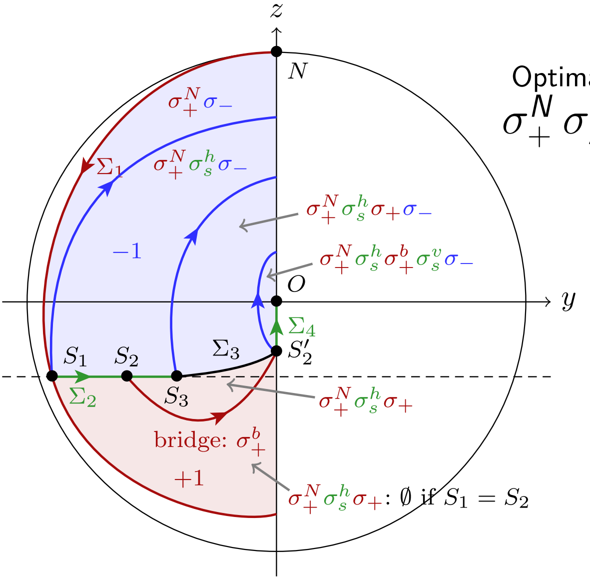


Case 2: S_1 exists and $S_2 \notin S_1S_3$



Case 3: S_1 doesn't exist

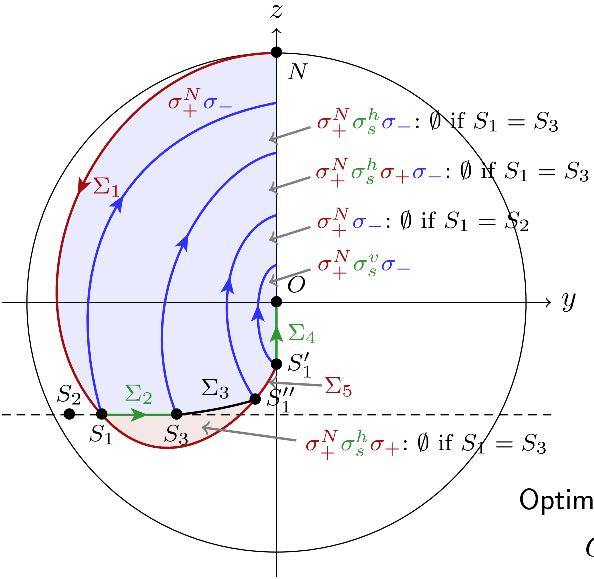
Case 1: S_1 exists and $S_2 \in S_1S_3$



Optimal trajectory from N to O:

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

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



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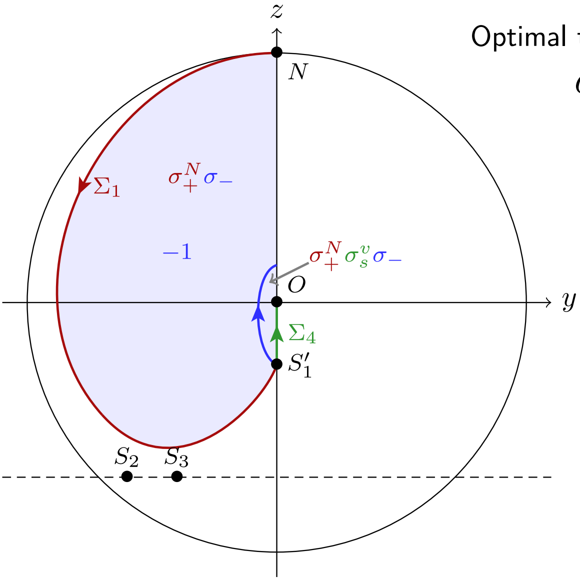


Optimal trajectory from N to O:

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

Theorem

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

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

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}	3.65×10^{-3}	42.685
C_2	2.464×10^{-2}	3.65×10^{-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

$$t_f = \inf_{u(\cdot)} \; T$$

$$\dot{x}(t) = f(x(t), u(t)),$$

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

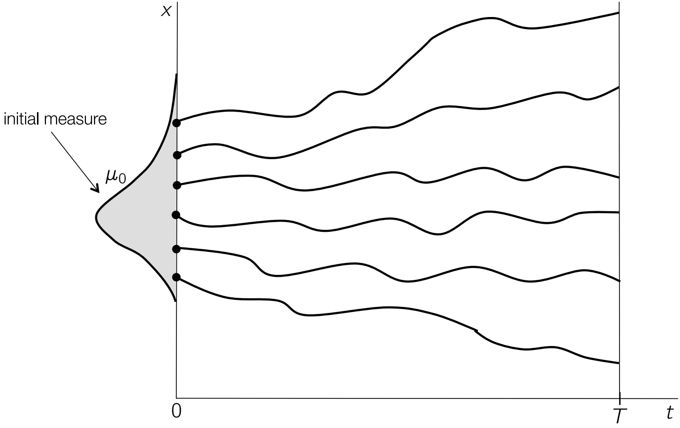
X, U, X_0, X_T are subsets of $\mathbb{R}^n$ which can be written as

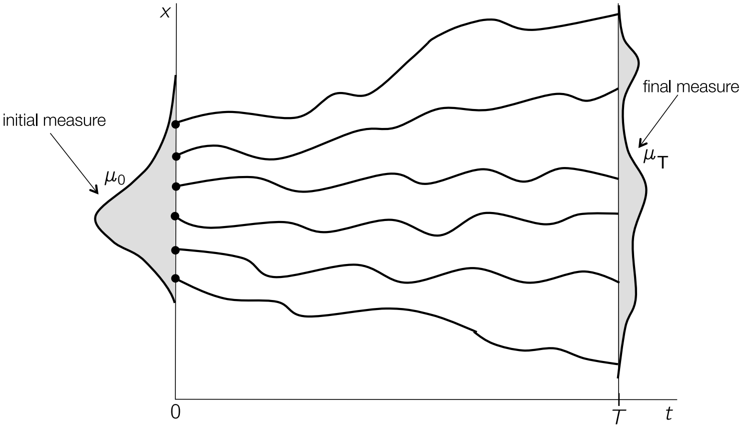
$$X = \{(t,x) : p_k(t,x) \geq 0,\ k = 0, \ldots, n_X\},\ U = \{u : q_k(u) \geq 0,\ k = 0, \ldots, n_U\}$$

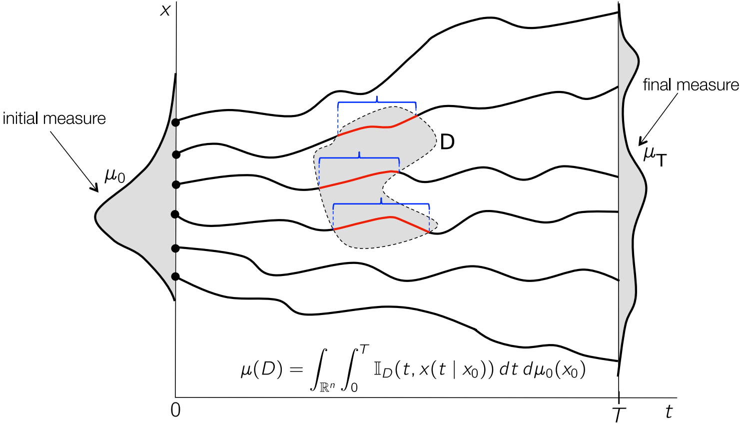
$$X_0 = \{x : r_k^0(x) \geq 0,\ k = 0, \ldots, n_0\},\ X_T = \{(t,x) : r_k^T(t,x)0,\ k = 0, \ldots, n_T\}$$

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:**

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

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- **Linear Problem on measures:**

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

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

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

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`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:

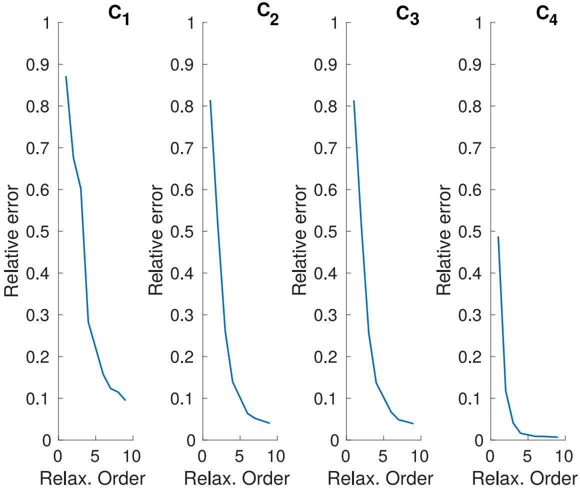
$$
\begin{aligned}
T_{SDP} = \min_{y^{\mu},\, y^{\mu_T}} \; & l_{y^{\mu_T}}(1) \\
& l_{y^{\mu}}\left(\frac{\partial v}{\partial t} + \frac{\partial v}{\partial x} f(x,u)\right) = l_{y^{\mu_T}}(v(\cdot, x_T)) - l_{y^{\mu_0}}(v(0, x_0)),\ \forall v \in \mathbb{R}[t,x], \\
& M_d(y^{\mu}) \succeq 0,\ M_d(g_i\,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

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.