Méthodes algébriques pour le contrôle optimal en Imagerie à Résonance Magnétique

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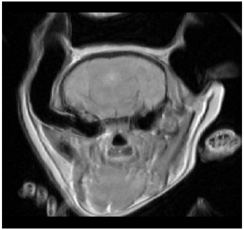
Contrast optimization for MRI

(N)MRI = (Nuclear) Magnetic Resonance Imagery

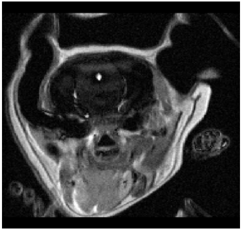
1. Apply a magnetic field to a body
2. Measure the radio waves emitted in reaction

Goal = optimize the contrast = distinguish two biological matters from this measure

Example: *in vivo* experiment on a mouse brain (brain vs parietal muscle)[1]



Bad contrast (not enhanced)



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[1] Éric Van Reeth et al. (2016). 'Optimal Control Design of Preparation Pulses for Contrast Optimization in MRI'. . In: Submitted IEEE transactions on medical imaging.

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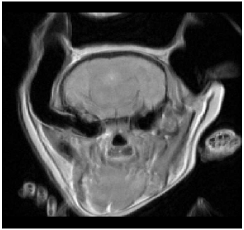

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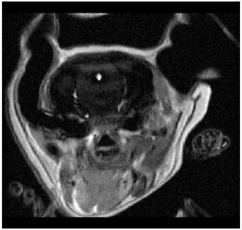

Good contrast (enhanced)

Known methods:

- inject contrast agents to the patient: potentially toxic...
- enhance the contrast dynamically $\Longrightarrow$ optimal control problem

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The Bloch equations for a single spin

The Bloch equations

$$\begin{cases} \dot{y} & = -\Gamma y - uz \\ \dot{z} & = \gamma(1-z) + uy \end{cases} \quad \rightsquigarrow \quad \dot{q} = F(\gamma, \Gamma, q) + uG(q)$$

- $q = (y, z)$: state variables
- γ, Γ: relaxation parameters (constants depending on the biological matter)
- u: control function (the unknown of the problem)

Physical limitations

- State variables: the Bloch Ball

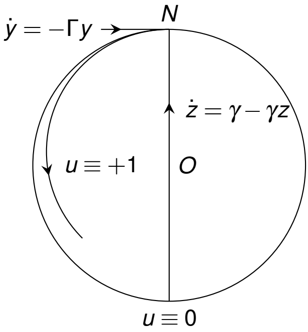
$$y^2 + z^2 \leq 1$$

- Parameters:

$$2\gamma \geq \Gamma > 0$$

- Control:

$$-1 \leq u \leq 1$$



Optimal control problems

Bloch equations for 2 spins: $\begin{cases} \dot{q}_1 = & F_1(\gamma_1, \Gamma_1, q_1) + uG_1(q_1) \\ \dot{q}_2 = & F_2(\gamma_2, \Gamma_2, q_2) + uG_2(q_2) \end{cases}$

Contrast problem

- Two matters, 4 parameters $\gamma_1, \Gamma_1, \gamma_2, \Gamma_2$
- Both spins have the same dynamic: $F_1 = F_2 = F$, $G_1 = G_2 = G$
- Equations

$$\begin{cases} \dot{q}_1 & = F(\gamma_1, \Gamma_1, q_1) + uG(q_1) \\ \dot{q}_2 & = F(\gamma_2, \Gamma_2, q_2) + uG(q_2) \end{cases}$$

- Goal: saturate #1, maximize #2:

$$\begin{cases} y_1 = z_1 = 0 \\ \text{Maximize } |(y_2, z_2)| \end{cases}$$

Multi-saturation problem

- Two spins of the same matter: $\Gamma_1 = \Gamma_2 = \Gamma$, $\gamma_1 = \gamma_2 = \gamma$
- Small perturbation on the second spin: $F_1 = F_2 = F$, $G_2 = (1 - \varepsilon)G_1$
- 2 parameters + ε
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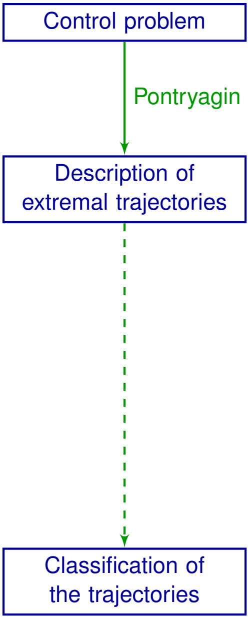

$$\dot{q} = F(\gamma, \Gamma, q) + uG(q)$$

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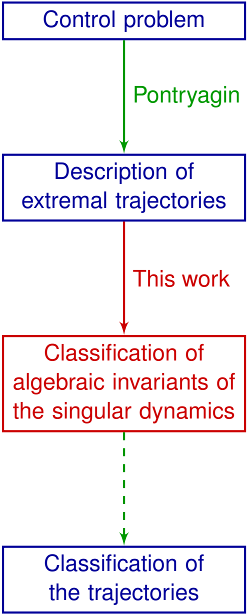
  $\dot{X} = D\,F - D'\,G$

Workflow



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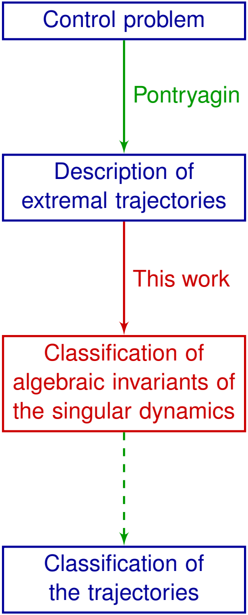

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Problem: study and classif. of the solutions of systems of polynomial equations

Method: exact algorithmic tools

Example: control of a single spin[2]

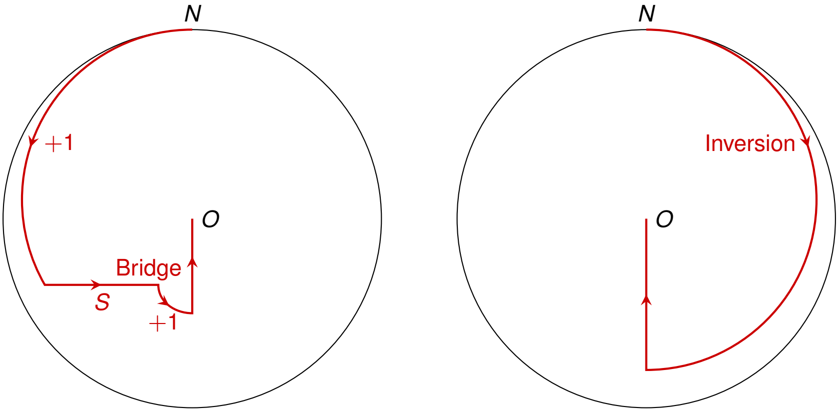

Figure: Time-minimal saturation for a single spin: left: $2\Gamma < 3\gamma$, right: $2\Gamma \geq 3\gamma$

Horizontal line at altitude $\dfrac{\gamma}{2(\Gamma - \gamma)}$ = part of the singular locus of $\{D = 0\}$

[2] Marc Lapert (2011). 'Développement de nouvelles techniques de contrôle optimal en dynamique quantique : de la Résonance Magnétique Nucléaire à la physique moléculaire'. PhD thesis. Université de Bourgogne, Dijon, France.

Polynomial tools: factorization and elimination

Factorization (isolation of components)

- Ex: $P = {X_1}^2 X_2 + 4 X_1 {X_2}^2 + 4 {X_2}^3 + {X_1}^2 + 4 X_1 X_2 + 4 {X_2}^2 \rightarrow (X_1 + 2 X_2)^2 (1 + X_2)$
- Very fast, efficiently implemented in most CAS
- Ex. square-free form: $\sqrt{P} := (X_1 + 2 X_2)(1 + X_2)$ has the same zeroes as P

Elimination (projection)

- Ex: $P_1 = X_1 + X_3$, $P_2 = X_1 X_2 + 2 X_3$
  $\rightarrow X_2 P_1 - P_2 = X_1 X_2 + X_2 X_3 - X_1 X_2 - 2 X_3$ (X_1 was eliminated)
- Computationally expensive, many different tools: resultants, Gröbner bases...
- Ex. saturation: $\langle f_1, \ldots, f_r : f^\infty \rangle = \langle f_1, \ldots, f_r, U f - 1 \rangle \cap \mathbb{Q}[X_1, \ldots, X_n]$
  The roots of this system "are" the roots of $f_1, \ldots, f_r$, minus the zeroes of f

Typical example of simplification

If I contains $P = fg$, we can split the study into:

1. the roots of $I + \langle f \rangle$
2. the roots of $I + \langle g \rangle$ saturated by f

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Examples for multi-saturation

$$\begin{cases} \dot{q}_1 & = D\,F(\gamma, \Gamma, q_1) - D'\,G(q_1) \\ \dot{q}_2 & = D\,F(\gamma, \Gamma, q_2) - D'\,(1-\varepsilon)G(q_2) \end{cases}$$

Singularities of $\{D = 0\}$

- North pole
- Line defined by $\begin{cases} y_1 = (1-\varepsilon)y_2 \\ z_1 = z_2 = z_S := \frac{\gamma}{2(\Gamma-\gamma)} \end{cases}$ (cf. the horizontal line for a single spin)

Equilibrium points $D = D' = 0$

- Horizontal plane $z_1 = z_2 = z_S = \frac{\gamma}{2(\Gamma-\gamma)}$
- Vertical line $y_1 = y_2 = 0$, $z_1 = z_2$
- 3 more complicated surfaces (related to the colinearity loci)

We can fully describe all invariants!

Previous results for the contrast problem[3]

Study of 4 experimental cases:

Matter #1 / # 2	γ_1	Γ_1	γ_2	Γ_2
Water / cerebrospinal fluid	0.01	0.01	0.02	0.10
Water / fat	0.01	0.01	0.15	0.31
Deoxygenated / oxygenated blood	0.02	0.62	0.02	0.15
Gray / white brain matter	0.03	0.31	0.04	0.34

Separated by means of several invariants:

- Number of singularities of $\{D = 0\}$ $\rightsquigarrow$ Always 1 for water?
- Structure of $\{D = D' = 0\}$
- Eigenvalues of the linearizations at equilibrium points
- Study of the quadratic approximations at points where the linearization is 0

[3] Bernard Bonnard, Monique Chyba, Alain Jacquemard and John Marriott (2013). 'Algebraic geometric classification of the singular flow in the contrast imaging problem in nuclear magnetic resonance'. In: *Mathematical Control and Related Fields* 3.4, pp. 397–432. ISSN: 2156-8472. DOI: 10.3934/mcrf.2013.3.397.

Classification for the contrast problem

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More complicated

- 4 variables, 4 parameters ($\rightsquigarrow$ 3 by homogeneity)
- Polynomials of high degree

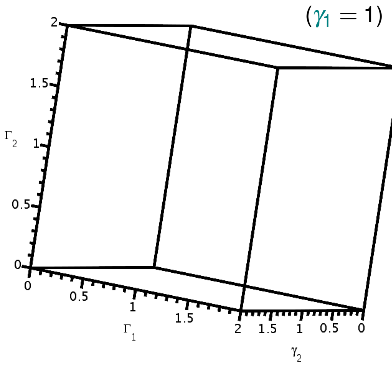
Singularities of $\{D = 0\}$ using Gröbner bases and factorisations/saturations

(After appropriate saturations) the ideal contains

$$\begin{cases} 0 & = P_{y_2}(y_2^2, \bullet) \text{ with degree 4 in } y_2^2 \text{ (8 roots)} \\ \bullet y_1 & = P_{y_1}(y_2, \bullet) \\ \bullet z_1 & = P_{z_1}(y_2, \bullet) \\ \bullet z_2 & = P_{z_2}(y_2, \bullet) \\ & \vdots \end{cases}$$

$\Longrightarrow$ study of the number of roots of P_{y_2} (depending on its leading coefficient and discriminant)

Singularities of $\{D = 0\}$ for the contrast problem: first results



Properties:

- Finite number of singularities for each value of the parameters
- Singularities come in pairs: invariant under $(y_i \mapsto -y_i)$

Classification in terms of Γ_i, γ_i:

- Generically: 4 pairs of singularities
- 3 pairs on a surface with several components:
  - one hyperplane
  - one quadric
  - one degree 24 surface
  - ...
- 2 pairs on a curve with many components
- 1 pair on a set of points

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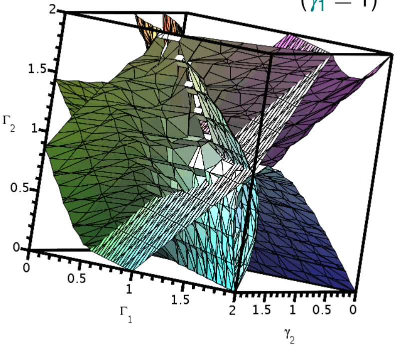
$(\gamma_1 = 1)$



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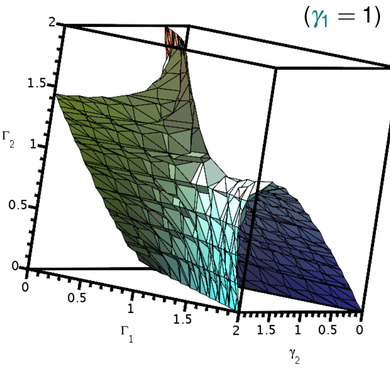

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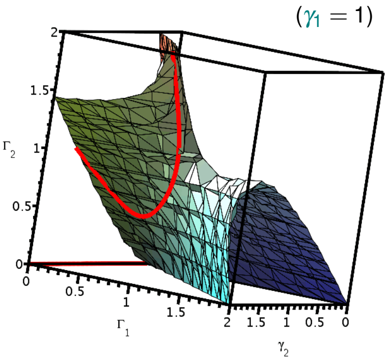

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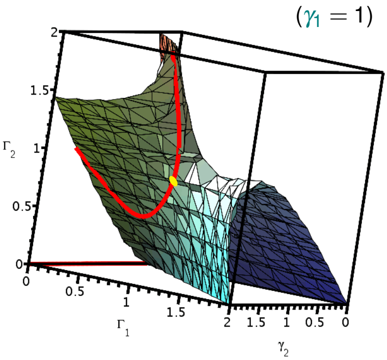

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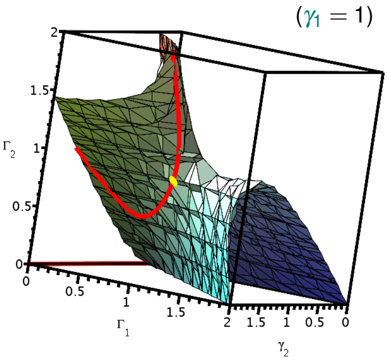

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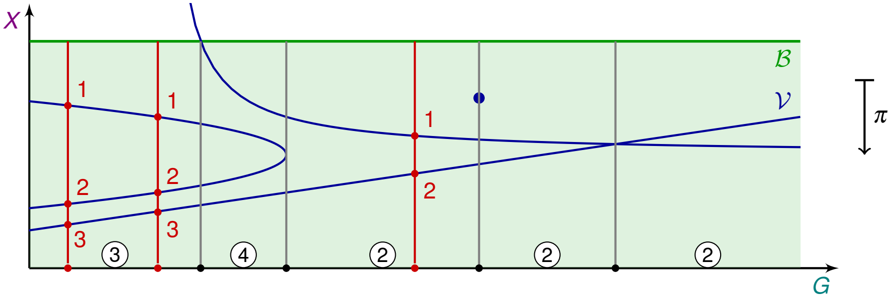
Can we get more information? For example, information about real points?

The real roots classification problem: state of the art and contribution



Real Roots Classification problem

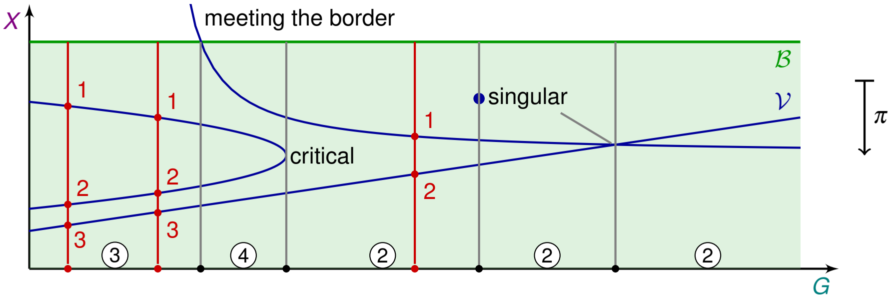
Goal: Partition of the parameter space s.t. $\#\left(\mathcal{V}\cap\mathcal{B}\cap\pi^{-1}(g)\right) = \text{constant}$

- $\mathcal{V} = \{D = \frac{\partial D}{\partial y_1} = \frac{\partial D}{\partial z_1} = \frac{\partial D}{\partial y_2} = \frac{\partial D}{\partial z_2} = 0\}$
- $\mathcal{B}$: Bloch ball

Existing tools

- Cylindrical Algebraic Decomposition
- Specific tools for roots classification
- Unable to solve the MRI problem

$\rightarrow$ Can we exploit the determinantal structure?



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Contribution[4]

- Dedicated strategy for the structure
- Refines existing strategies (easy to implement)
- Able to solve the MRI problem

[4] Bernard Bonnard, Jean-Charles Faugère, Alain Jacquemard, Mohab Safey El Din and Thibaut Verron (2016). 'Determinantal sets, singularities and application to optimal control in medical imagery'. In: *Proceedings of the 2016 International Symposium on Symbolic and Algebraic Computation*. ISSAC '16. Waterloo, Canada

Application to the contrast problem

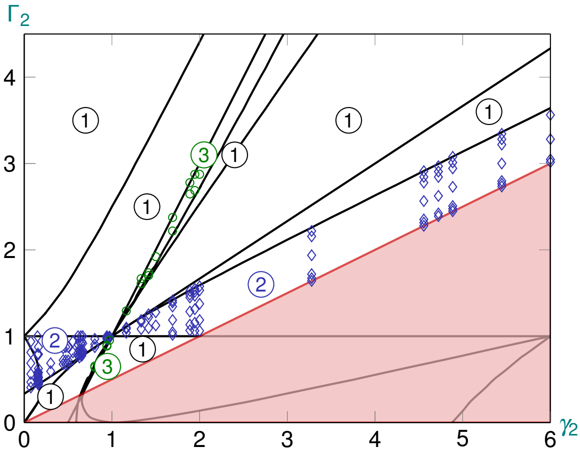
Full classification strategy

1. Real Roots Classification → limits of the cells
2. Cylindrical algebraic decomposition → points in each cell
3. Gröbner basis computations for each point → count of singularities

- Results obtained with Maple, using the `FGb` Gröbner basis library for eliminations
- Source code and full results available at `mercurey.gforge.inria.fr`

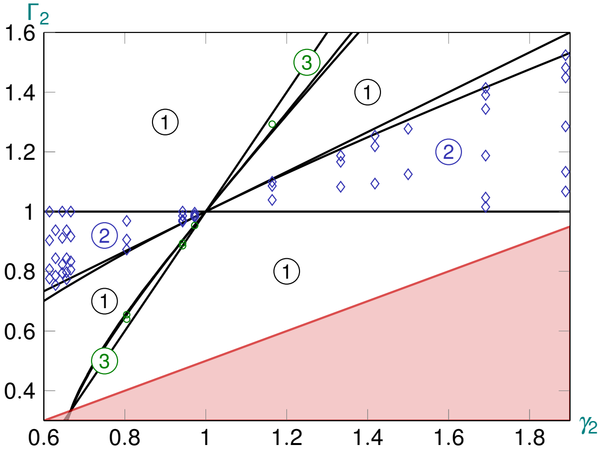
Case	# Params	Time for step 1 (direct)	Time for step 1 (new strat.)	Results	Time for step 2	# Points
Water	2	110 s	10 s	9 pols. (deg $\leq$ 3)	50 s	1533
General	3	>24 h	2 h	14 pols. (deg $\leq$ 14)	48 h	10 109

Detailed results for the contrast problem in the case of water



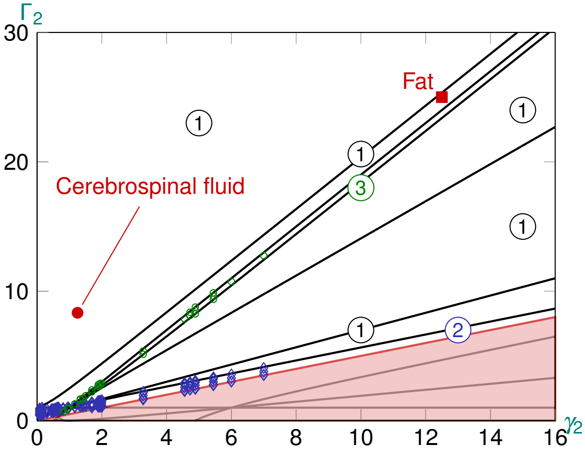
- Case of water: 1, 2 or 3 singular points
- General case: 1, 2, 3, 4 or 5 singular points

Detailed results for the contrast problem in the case of water (zoom in)



- Case of water: 1, 2 or 3 singular points
- General case: 1, 2, 3, 4 or 5 singular points

Detailed results for the contrast problem in the case of water (zoom out)



- Case of water: 1, 2 or 3 singular points
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Conclusion and perspectives

This work

- Applications of algebraic methods to an optimal control problem
- Dedicated strategy for a classification problem related to one of the invariants

Perspectives

Algorithmically:

- Extension of the algorithms to structures of other invariants

And for the MRI problem:

- Direct relation between the invariants and properties of the trajectories?
- Is it possible to lift some approximations?
- Further studies, *e.g.* classification according to optimal contrast

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Thank you for your attention!