Algebraic classification methods for an optimal control problem in medical imagery

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Contrast optimization for MRI

(N)MRI = (Nuclear) Magnetic Resonance Imagery

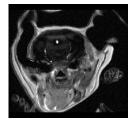
- 1. Apply a magnetic field to a body
- 2. Measure the radio waves emitted in reaction

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)



Good contrast (enhanced)

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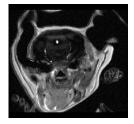
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Known methods:

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

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Problem and results

Study of optimal control strategy for the MRI

- Optimal control theory: find settings for the MRI device ensuring e.g. good contrast
- Already proved to give better results than implemented heuristics²
- Powerful tools allow to understand the control policies

These questions reduce to algebraic problems

- Invariants of a group action on vector fields
- Algebraic: rank conditions, polynomial equations, eigenvalues...

Contribution: algebraic tools for this workflow

- Demonstrate use of existing tools
- Dedicated strategies for specific problems (real roots classification) adapted to the structure of the systems (determinantal systems)
- These structures extend beyond the MRI problem

²Marc Lapert, Yun Zhang, Martin A. Janich, Steffen J. Glaser and Dominique Sugny (2012). 'Exploring the Physical Limits of Saturation Contrast in Magnetic Resonance Imaging'. In: *Scientific Reports* 2.589.

1. Context and problem statement

- Magnetic Resonance Imagery
- Physical modelization of the problem

2. Optimal control theory

- What is control theory?
- Pontryagin's Maximum principle
- Study of singular extremals: algebraic questions

3. General algebraic techniques

- Tools for polynomial systems
- Examples of results

4. Real roots classification for the singularities of determinantal systems

- What is the goal?
- State of the art and main results
- General strategy: what do we need to compute?
- Dedicated strategy for determinantal systems
- Results for the contrast problem

5. Conclusion

The Bloch equations

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

- 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

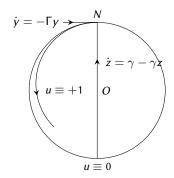
$$y^2 + z^2 \le 1$$

Parameters:

$$2\gamma \ge \Gamma > 0$$

Control:

 $-1 \leq \mathbf{u} \leq 1$



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 γ_1 , Γ_1 , γ_2 , Γ_2
- Both spins have the same dynamic: $F_1 = F_2 = F$, $G_1 = G_2 = G$
- Equations

$$\dot{q}_1 = F(\gamma_1, \Gamma_1, q_1) + uG(q_1)$$

 $\dot{q}_2 = F(\gamma_2, \Gamma_2, q_2) + uG(q_2)$

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
- Equations:

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

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What is control theory?

Controlled system:

$$\begin{cases} \dot{q}(t) = \mathcal{F}(q(t), u(t), t) \\ q(0) = q_0 & \text{(or more general constraints)} \end{cases}$$

Control theory = answer one of the following questions for such a system:

- Accessibility Given *V*, is there a control u such that $q(t_f) \in V$ for some t_f ? More generally, what is the set of accessible points?
 - Optimality What is the shortest time in which we can reach a target set? More generally, minimize a combination of a running cost (Lagrange cost, *e.g.* energy):

$$C_{L}(\boldsymbol{u}) = \int_{0}^{t_{f}} f^{0}(q(t), \boldsymbol{u}(t), t) \mathrm{d}t$$

and a terminal cost (Mayer cost, e.g. time):

$$C_{\mathcal{M}}(\boldsymbol{u}) = g(q(t_f), t_f)$$

Interlude 1: different settings, different problems?

$$\left\{ egin{aligned} \dot{q}(t) &= \mathcal{F}(q(t), \mathbf{u}(t), t) \ q(0) &= q_0 \end{aligned}
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Many different settings ...

- ▶ Is the system autonomous? (Or does *F* depend on *t*?)
- ▶ Is the cost evaluated at *t*_{*f*}, or all along the trajectory?
- ... and two kinds of questions
 - What is the reachable set?
 - What is the cost of reaching a given set?

All of these questions are actually equivalent

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Pontryagin's Maximum principle

Optimal control problem: minimize $\int f^0(q, \mathbf{u})$ under the constraint $\dot{q} = F(q, \mathbf{u})$ ($q(t) \in \mathbb{R}^n$)

For finite-dimensional optimization, we have Lagrange multipliers. For control theory, we have...

Hamiltonian

Introduce multipliers $p = (p_1, \ldots, p_n) : \mathbb{R} \to \mathbb{R}^n$.

The Hamiltonian associated with the control problem is defined as

$$H(q, p, \boldsymbol{u}) := \langle p, F(q, \boldsymbol{u}) \rangle - f^0(q, \boldsymbol{u})$$

Pontryagin's Maximum principle

If u is an optimal control, then q, p and u are solutions of

$$\begin{cases} \dot{q} = \frac{\partial H}{\partial p} \\ \dot{p} = -\frac{\partial H}{\partial q} \end{cases}$$

and almost everywhere in t, u(t) maximizes the Hamiltonian:

$$H(q(t), p(t), u(t)) = \max_{v \in [-1,1]} H(q(t), p(t), v)$$

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The affine case: bang and singular arcs

The Bloch equations form an affine control problem:

 $\dot{q} = F(q) + {}^{u}G(q)$

Pontryagin's principle, the affine case

The control u maximizes over [-1, 1]:

$$H(q, p, u) = H_F(q, p) + uH_G(q, p).$$

Two situations:

►
$$H_G \neq 0 \implies u = \operatorname{sign}(H_G)$$
: "Bang" arc

 $\blacktriangleright H_G = 0 \implies ???$

Singular trajectories for the Bloch equations

They satisfy $\dot{q} = DF(q) - D'G(q)$ with optimal control $u = \frac{D'}{D}$

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In practice one chooses u such that H_G remains 0: Singular arc

 \implies need bifurcation strategies...

Singular trajectories for the Bloch equations

They satisfy $\dot{q} = DF(q) - D'G(q)$ with optimal control $u = \frac{D'}{D}$.

What are D and D'?

For singular trajectories, we have 4 linear equations in p:

$$p \cdot F = 0$$
 "Exceptional" case

$$p \cdot G = 0$$
 Singular arc

$$p \cdot [G, F] = 0$$
 d/dt the previous one...

$$p \cdot ([[G, F], F] + u[[G, F], G]) = 0$$
 ... and again

Cramer's rule: the solution is

$$u = \frac{D'}{D}$$
 (exists iff $D \neq 0$)

where

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

D and *D'* are determinants of 4×4 matrices

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Interlude 2: Lie brackets and controllability of affine systems

Affine control problem: $\dot{q} = uF + vG$ (simpler case, no drift)

Question: What is
$$[F, G] = \frac{\partial G}{\partial q}F - \frac{\partial F}{\partial q}G$$
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It measures the interactions between the two controls!

Theorem (characterization of controllability)

The system is controllable at q (= we can go in any direction from q) if and only if dim Vect(F, G, [F, G], [[F, G], F], ...) = dimension of the ambient space

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Study of invariants

Group action on vector fields (F, G)

Control system: $\dot{q} = F(q) + uG(q)$

- Changes of coordinates: $q \leftarrow \varphi(q)$
- Feedback: $\boldsymbol{u} \leftarrow \alpha(\boldsymbol{q}) + \beta(\boldsymbol{q})\boldsymbol{v}$

Long-term goal: classification of the parameters via invariants of this group action

Example: control of a single spin³

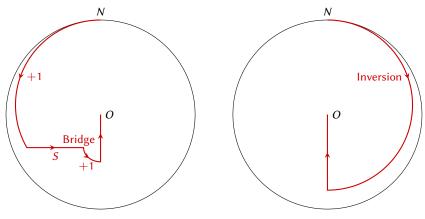


Figure: Time-minimal saturation for a single spin: left: $2\Gamma < 3\gamma$, right: $2\Gamma \ge 3\gamma$

³Marc 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.

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Examples of invariants (fixed values of the parameters)

- Hypersurface Σ : {D = 0}
- Singularities of Σ

...

- Set where F and G are colinear
- ▶ Set where *G* and [*F*, *G*] are colinear
- Equilibrium points: $\{D = D' = 0\}$
- Eigenvalues of the linearized system at equilibrium points (up to a constant)

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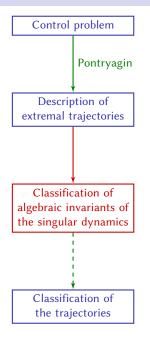
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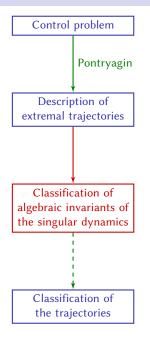
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Problem: study and classification of the solutions of systems of polynomial equations

Method: exact algorithmic tools

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Polynomial tools: factorization and elimination

Factorization

- Given $P \in \mathbb{Q}[X_1, \ldots, X_n]$, compute $F_i \in \mathbb{Q}[X_1, \ldots, X_n], \alpha_i \in \mathbb{N}$ such that $P = F_1^{\alpha_1} \cdots F_r^{\alpha_r}$
- Very fast, efficiently implemented in most CAS
- Ex. square-free form: $\sqrt{P} := F_1 \cdots F_r$ has the same zeroes as *P*

Elimination

- ▶ Given an ideal $I \subset \mathbb{Q}[X_1, \ldots, X_n]$ and $k \in \{1, \ldots, n\}$, compute $I \cap \mathbb{Q}[X_{k+1}, \ldots, X_n]$
- Computationally expensive, many different tools: resultants, Gröbner bases..
- ► Ex. saturation: $\langle f_1, \ldots, f_r \rangle$: $f^{\infty} = \langle f_1, \ldots, f_r, Uf 1 \rangle \cap \mathbb{Q}[X_1, \ldots, X_n]$ 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 $I + \langle f \rangle$
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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!

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 $\{D = 0\}$
- Structure of $\{D = D' = 0\}$
- Eigenvalues of the linearizations at equilibrium points
- > Study of the quadratic approximations at points where the linearization is 0

⁴Bernard 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

$$\begin{cases} \dot{q}_1 &= D F(\gamma_1, \Gamma_1, q_1) - D' G(q_1) \\ \dot{q}_2 &= D F(\gamma_2, \Gamma_2, q_2) - D' G(q_2) \end{cases}$$

More complicated

- ▶ 4 variables, 4 parameters (~→ 3 by homogeneity)
- Polynomials of high degree

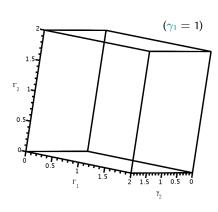
Singularities of $\{D = 0\}$ using Gröbner bases and factorisations/saturations

(After appropriate saturations) the ideal contains

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

Study of the leading coefficient and discriminant of P_{y_2}

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

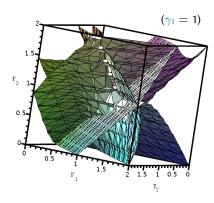


Properties:

- Finite number of singularities for each value of the parameters
- Singularities come in pairs: invariant under (y_i → −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

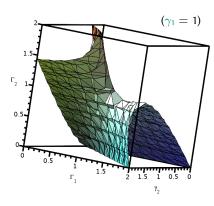


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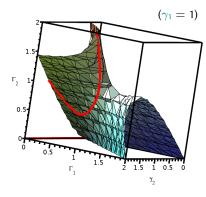


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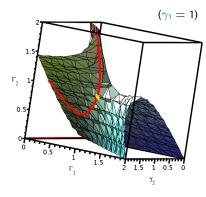
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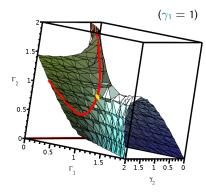
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Can we get more information? For example, information about real points?

1. Context and problem statement

- Magnetic Resonance Imagery
- Physical modelization of the problem

2. Optimal control theory

- What is control theory?
- Pontryagin's Maximum principle
- Study of singular extremals: algebraic questions

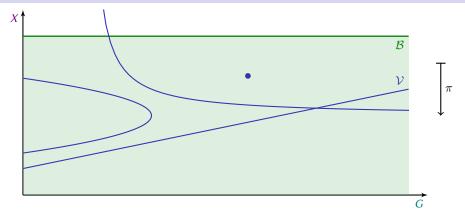
3. General algebraic techniques

- Tools for polynomial systems
- Examples of results

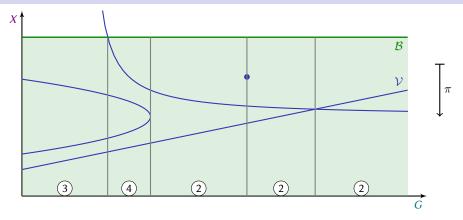
4. Real roots classification for the singularities of determinantal systems

- What is the goal?
- State of the art and main results
- General strategy: what do we need to compute?
- Dedicated strategy for determinantal systems
- Results for the contrast problem

5. Conclusion

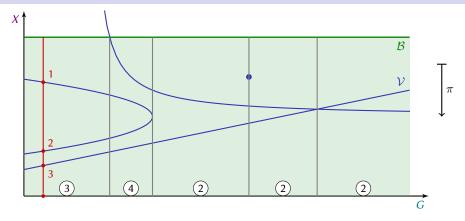


- Algebraic variety \mathcal{V} : singularities of Σ : $D = \frac{\partial D}{\partial y_1} = \frac{\partial D}{\partial y_2} = \frac{\partial D}{\partial z_1} = \frac{\partial D}{\partial z_2} = 0$
- ► Semi-algebraic constraints \mathcal{B} : Bloch Ball $y_i^2 + z_i^2 1 \le 0$



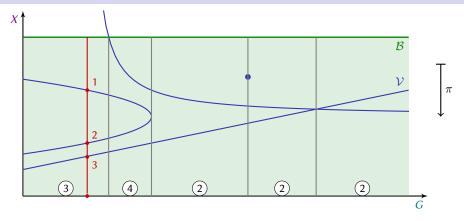
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Goal



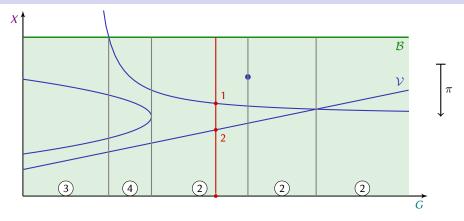
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Goal



- Algebraic variety \mathcal{V} : singularities of Σ : $D = \frac{\partial D}{\partial v_1} = \frac{\partial D}{\partial z_2} = \frac{\partial D}{\partial z_1} = \frac{\partial D}{\partial z_2} = 0$
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Goal

State of the art and main results

State of the art:

- General tool: Cylindrical Algebraic Decomposition Collins, 1975
- Specific tools for roots classification Yang, Hou, Xia, 2001 Lazard, Rouillier, 2007

Problem

- None of these algorithms can solve the problem efficiently:
 - 1050 s in the case of water $(\gamma_1 = \Gamma_1 = 1 \rightarrow 2 \text{ parameters})$
 - > 24 h in the general case (3 parameters)
- Can we exploit the determinantal structure to go further?

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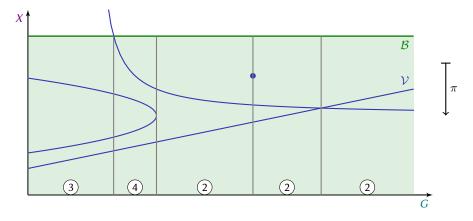
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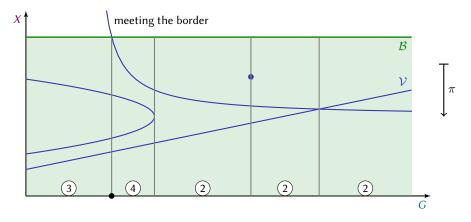
Main results

Bonnard, Faugère, Jacquemard, Safey, V., 2016

- Dedicated strategy for real roots classification for determinantal systems
- Can use existing tools for elimination
- Main refinements:
 - Rank stratification
 - Incidence varieties
- ► Faster than general algorithms:
 - 10 s in the case of water
 - 4 h in the general case
- Results for the application
 - Full classification
 - In the case of water: 1, 2 or 3 singularities
 - In the general case: 1, 2, 3, 4 or 5 singularities

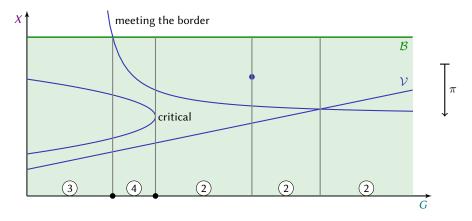


In our case, the only points where the number of roots may change are projections of:



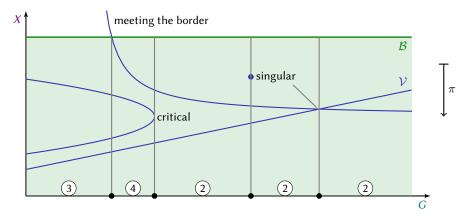
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• points where \mathcal{V} meets the border of the semi-algebraic domain



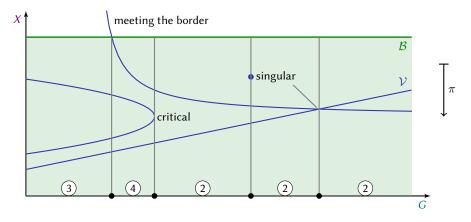
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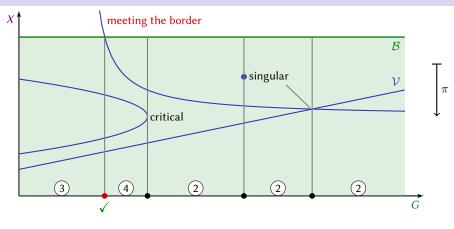


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 $=: K(\pi, \mathcal{V})$

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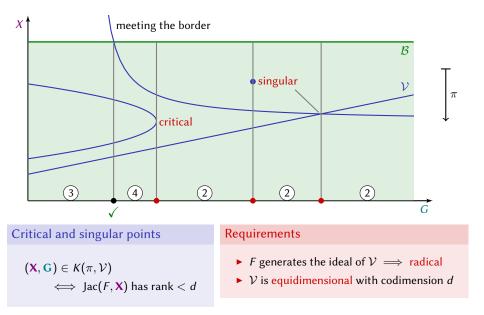
We want to compute $P \in \mathbb{Q}[G]$ with $P \neq 0$ and P vanishing at all these points



Intersection with the border

For each inequality f > 0 defining \mathcal{B}

- 1. Add f = 0 to the equations of \mathcal{V}
- 2. Compute the image of the variety through π (eliminate X)



- $A = k \times k$ -matrix filled with polynomials in *n* variables **X** and *t* parameters **G**
- $1 \le r < k$ target rank
- Determinantal variety: $V_{\leq r}(A) = \{(\mathbf{x}, \mathbf{g}) : \operatorname{rank}(A(\mathbf{x}, \mathbf{g})) \leq r\}$

Our system:
$$\mathcal{V} = \{ D = \frac{\partial D}{\partial y_1} = \frac{\partial D}{\partial y_2} = \frac{\partial D}{\partial z_1} = \frac{\partial D}{\partial z_2} = 0 \}$$

 \implies In terms of determinantal systems: $n = 4, k = 4, r = 3, \mathcal{V} = K(\pi, V_{\leq r}(M))$

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For a generic matrix A with the same parameters

- $V_{\leq r}(A)$ equidimensional with codimension $(k r)^2$
- Sing $(V_{\leq r}(A)) = V_{\leq r-1}(A)$, *t*-equidimensional
- Crit(π , $V_{\leq r}(A)$) has dimension < t
- ► Natural stratification : $K(\pi, V_{\leq r}(A)) = \text{Sing}(V_{\leq r}(A)) \cup \text{Crit}(\pi, V_{\leq r}(A))$

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For our specific matrix M

- $V_{\leq r-1}(M) \subset \mathcal{V}$ (always true: why?)
- $V_{\leq r-1}(M)$ is equidimensional with dimension *t*
- $\mathcal{V} \smallsetminus V_{\leq r-1}(\mathcal{M})$ has dimension < t
- ▶ Rank stratification : $\mathcal{V} = (\mathcal{V} \cap V_{\leq r-1}(M)) \cup (\mathcal{V} \setminus V_{\leq r-1}(M))$

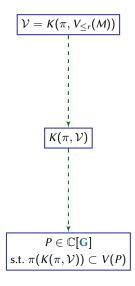
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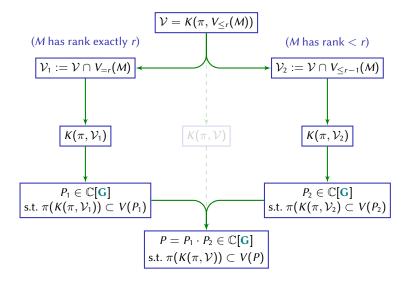
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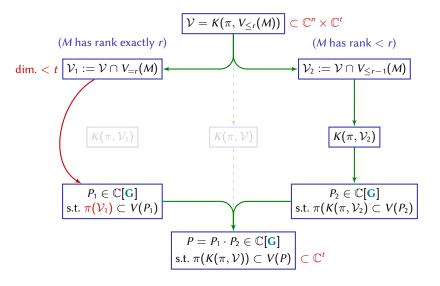
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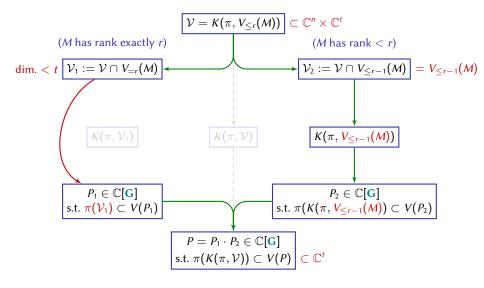




Rank stratification



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We can model $V_{\leq r}$ (*e.g.* with minors), but how to enforce equality?

$$V_{=r} = V_{\leq r} \smallsetminus V_{\leq r-1}$$

We would like to saturate, but how?

We use a local description: For each *r*-minor *A* of *M*, we consider the ideal:

 $I(V_{\leq r}) + \langle U \cdot \det(A) - 1 \rangle \cap \mathbb{Q}[X, G]$

which is generated by the (r + 1)-minors of M containing A.

We can model $V_{< r}$ (*e.g.* with minors), but how to enforce equality?

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Interlude 3: Cramer's rule and Schur complement

Cramer's rule / Gauß elimination (A is invertible)

$$k - 1 \int \left[\begin{array}{c} A & B \\ 1 \int \left[\begin{array}{c} C & d \\ K - 1 \end{array} \right] = \left[\begin{array}{c} I_{k-1} & 0 \\ \bullet & 1 \end{array} \right] \cdot \left[\begin{array}{c} A & 0 \\ 0 & d - CA^{-1}B \end{array} \right] \cdot \left[\begin{array}{c} I_{k-1} & \bullet \\ 0 & 1 \end{array} \right]$$
$$d - CA^{-1}B = \frac{\det(M)}{\det(A)}$$

Schur complement (A is invertible)

$$r \uparrow \begin{bmatrix} A & B \\ R & r \uparrow \end{bmatrix} = \begin{bmatrix} I_r & 0 \\ \bullet & I_{k-r} \end{bmatrix} \cdot \begin{bmatrix} A & 0 \\ 0 & D - CA^{-1}B \end{bmatrix} \cdot \begin{bmatrix} I_r & \bullet \\ 0 & I_{k-r} \end{bmatrix}$$

(i, j)-entry of $D - CA^{-1}B = \frac{\det((r+1)-\min(A + \operatorname{rowcol}(r+i, r+j)))}{\det(A)}$

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Modelization using incidence varieties

Reminder: k = size of the matrix; r = target rank

Possible modelizations for determinantal varieties

- Minors: rank(A) $\leq r \iff$ all r + 1-minors of A are 0
- ▶ Incidence system: $rank(A) \le r \iff \exists L, A \cdot L = 0$ and rank(L) = k r

Minors:

- $\binom{k}{r+1}^2$ equations
- Codimension $(k r)^2$

Incidence system:

- k(k r) new variables (entries of the matrix *L*)
- $(k-r)^2 + k(k-r)$ equations
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- ▶ Codimension (k − r)²

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- Codimension: $(k r)^2 + k(k r)$

Properties of the incidence system (generically and in our situation)

- ► It forms a regular sequence (codimension = length) ⇒ equidimensional
- It defines a radical ideal

Consequence for the strategy

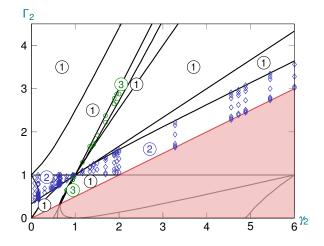
 $K(\pi, V_{\leq r-1}(M))$ can be computed with the incidence system, using maximal minors of the Jacobian matrix

Application to the contrast problem (benchmarks)

- Computations run on the matrix of the contrast optimization problem
 - Water: $\Gamma_1 = \gamma_1 = 1 \implies 2$ parameters
 - General: $\gamma_1 = 1 \implies 3$ parameters
- Results obtained with Maple
- Source code and full results available at mercurey.gforge.inria.fr

Elimination tool	Water (direct)	Water (det. strat.)	General (direct)	General (det. strat.)
Gröbner bases (FGb)	100 s	10 s	>24 h	$46\times 200\text{s}$
Gröbner bases (F5)	-	1 s	-	110 s
Regular chains (RegularChains)	1050 s	-	>24 h	$90 imes 200 \mathrm{s}$

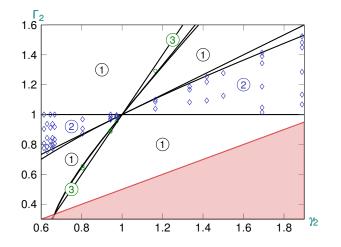
Results for the contrast problem in the case of water



Finishing the computations:

- 1. Classification algorithm \rightarrow limits of the cells
- 2. Cylindrical algebraic decomposition \rightarrow points in each cell
- 3. Gröbner basis computations for each point \rightarrow count of singularities

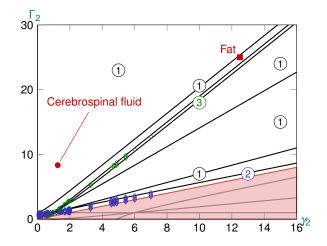
Results for the contrast problem in the case of water (zoom in)



Finishing the computations:

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



Finishing the computations:

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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

The end?

