Méthodes algébriques pour le contrôle optimal en Imagerie à Résonance Magnétique

Bernard Bonnard[1,2] Jean-Charles Faugère[3] Alain Jacquemard[1]
Jérémy Rouot[4] Mohab Safey El Din[3] Thibaut Verron[5]

1. Université de Bourgogne-Franche Comté, Dijon
2. Inria Sophia Antipolis, Équipe McTAO
3. UPMC Paris Sorbonne Universités, Inria Paris, CNRS, LIP6, Équipe PolSys
4. LAAS, CNRS, Toulouse
5. Toulouse Universités, INP-ENSEEIHT-IRIT, CNRS, Équipe APO

Séminaire Calcul Formel, Limoges

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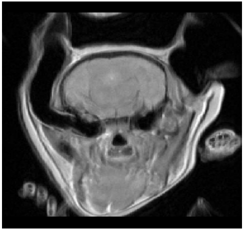
(N)MRI = (Nuclear) Magnetic Resonance Imagery

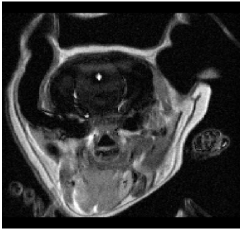
1. Apply a magnetic field to a body
2. Measure the radio waves emitted in reaction

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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Contrast optimization for MRI

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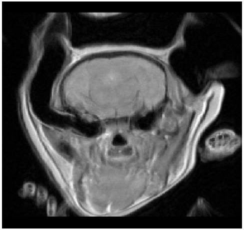

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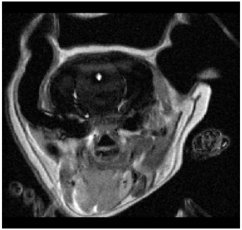

Good contrast (enhanced)

Known methods:

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

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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 heuristics[2]
- 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

[2] Marc 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.

Outline of the talk

1. Context and problem statement
    - Magnetic Resonance Imagery
    - Physical modelization of the problem

2. Optimal 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 for a single spin

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

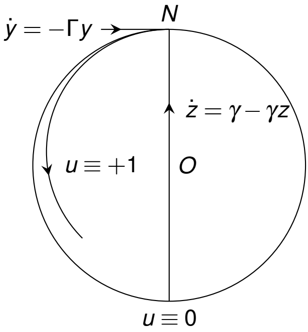
$$y^2 + z^2 \leq 1$$

- 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:

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

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:

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Outline of the talk

Pontryagin's Maximum principle

Control problem: minimize $C(q(t_f))$ under the constraint $\dot{q} = F(q,u)$ $(q(t) \in \mathbb{R}^n)$

Definition: 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

$$H(q,p,u) := \langle p, F(q,u) \rangle - C(q(t_f))$$

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:

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

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:

- $H_G \neq 0 \implies u = \text{sign}(H_G)$: "Bang" arc
- $H_G = 0 \implies$???

Singular trajectories for the Bloch equations

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

D and D' are determinants of 4×4 matrices (Cramer's rule for a linear system in p)

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

  $\implies$ need bifurcation strategies...

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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: $u \leftarrow \alpha(q) + \beta(q)v$

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

Example: control of a single spin[3]

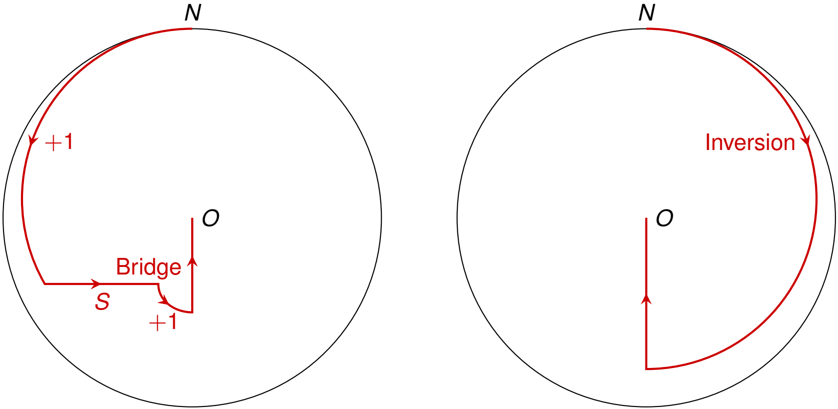

Figure: Time-minimal saturation for a single spin: left: $2\Gamma < 3\gamma$, right: $2\Gamma \geq 3\gamma$

[3] 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.

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Examples of invariants (fixed values of the parameters)

- Hypersurface $\Sigma : \{D = 0\}$
- 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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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: $\langle f_1, \ldots, f_r : f^\infty \rangle = \langle f_1, \ldots, f_r, Uf - 1 \rangle \cap \mathbb{Q}[X_1, \ldots, X_n]$
  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 $I + \langle f \rangle$
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[4]

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

[4] 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

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

More complicated

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

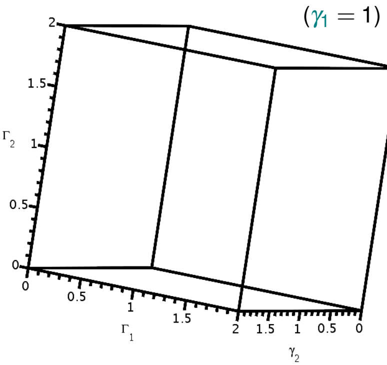
Singularities of $\{D = 0\}$ using Gröbner bases and factorisations/saturations

(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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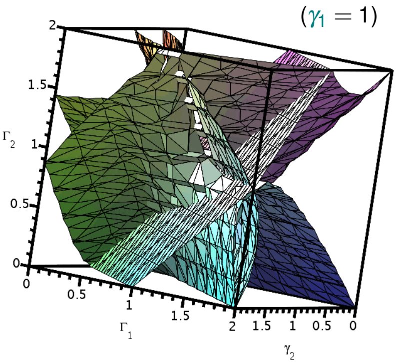

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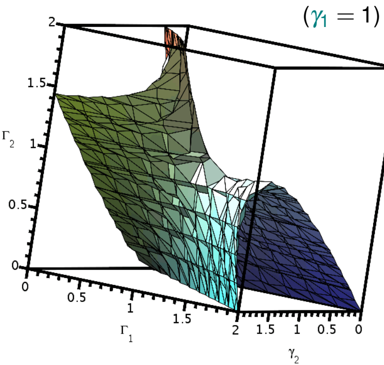

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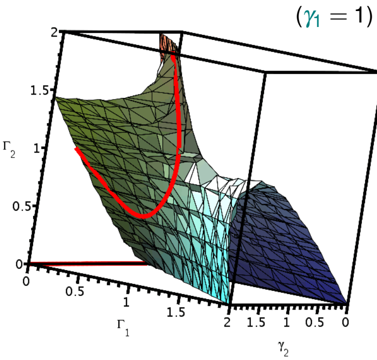

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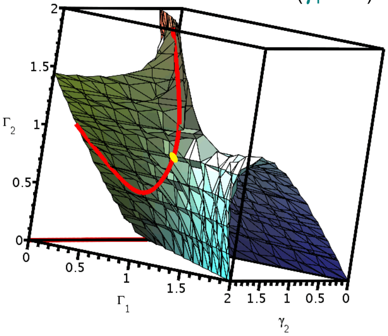
Singularities of $\{D = 0\}$ for the contrast problem: first results

$(\gamma_1 = 1)$



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
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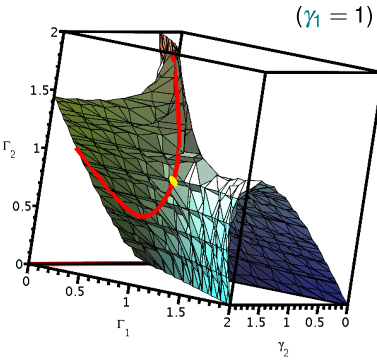

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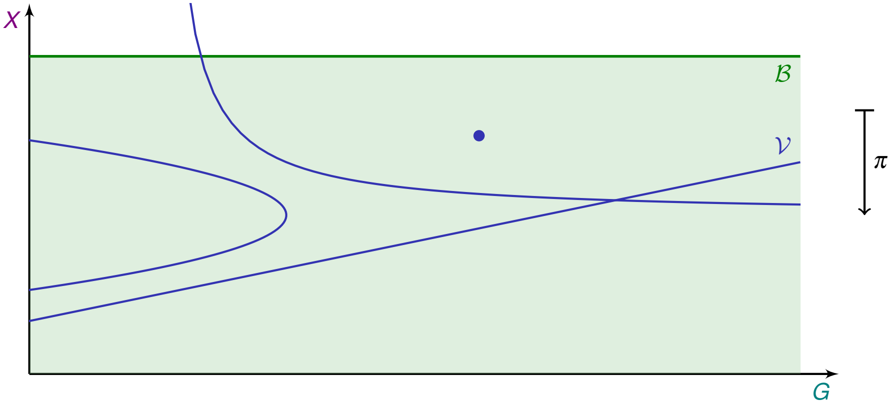
Can we get more information? For example, information about real points?

Outline of the talk

1. Context and problem statement
   - Magnetic Resonance Imagery
   - Physical modelization of the problem
2. Optimal 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 goal : real roots classification



- 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 $y_i^2 + z_i^2 - 1 \leq 0$

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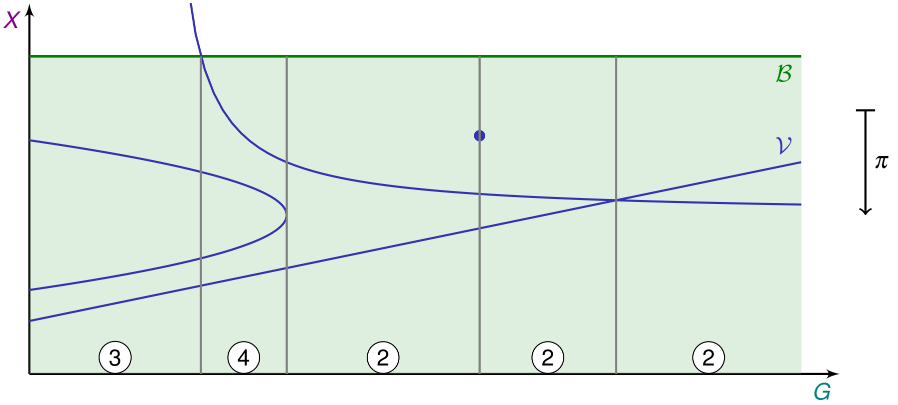

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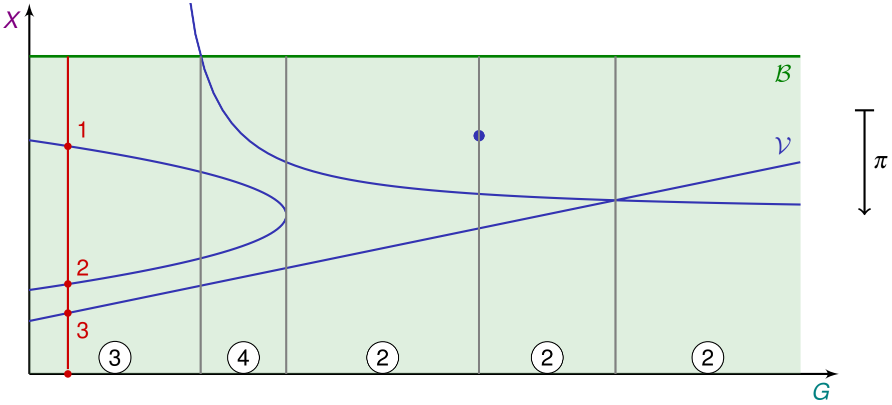
Partition of the parameter space depending on the number of points of $\mathcal{V} \cap \mathcal{B}$ above

The goal : real roots classification



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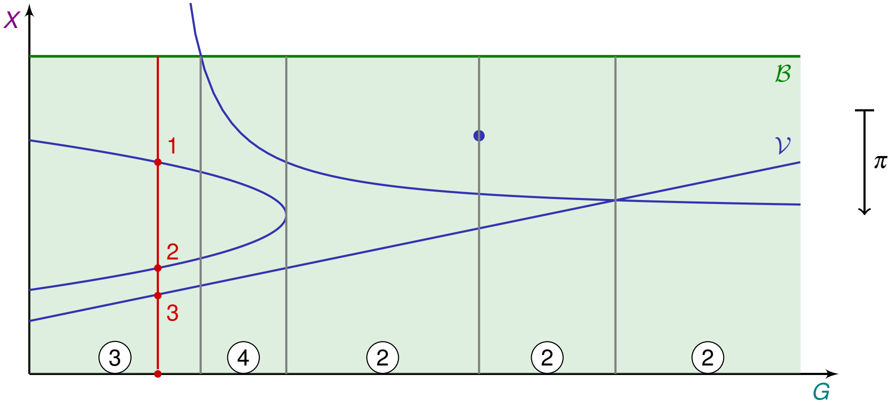

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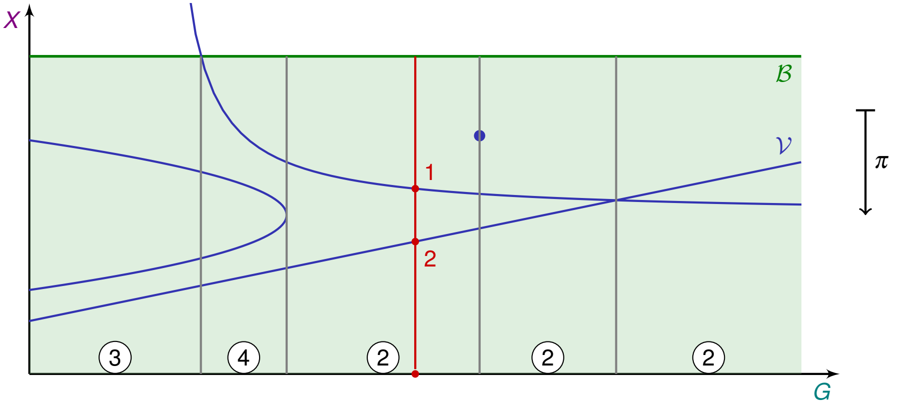

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State of the art and main results

State of the art:

- General tool: Cylindrical Algebraic Decomposition
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- None of these algorithms can solve the problem efficiently:
  - 1050 s in the case of water ($\gamma_1 = \Gamma_1 = 1 \to 2$ parameters)
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- Dedicated strategy for real roots classification for determinantal systems
- Can use existing tools for elimination
- Main refinements:
  - Rank stratification
  - Incidence varieties

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Main results

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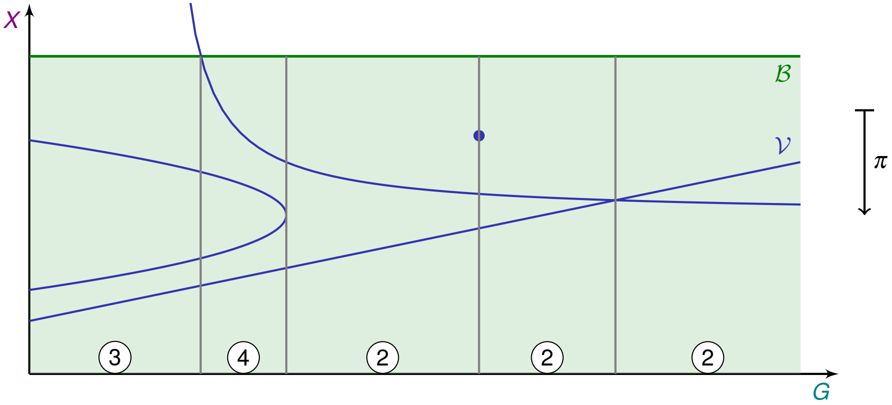
- Faster than general algorithms:
  - 10 s in the case of water
  - 4 h in the general case
- Results for the application
  - Full classification
  - In the case of water: 1, 2 or 3 singularities
  - In the general case: 1, 2, 3, 4 or 5 singularities

General strategy for the real roots classification problem



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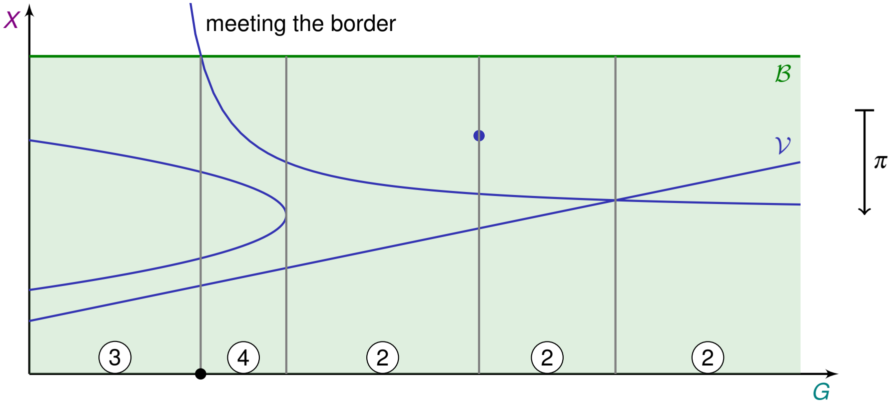

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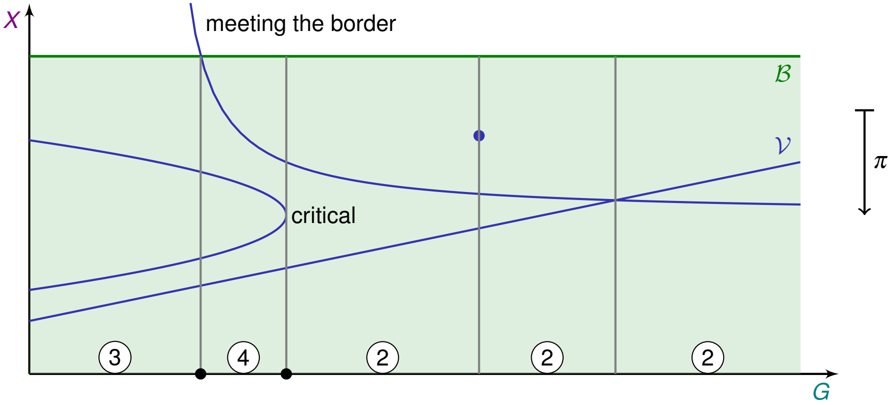

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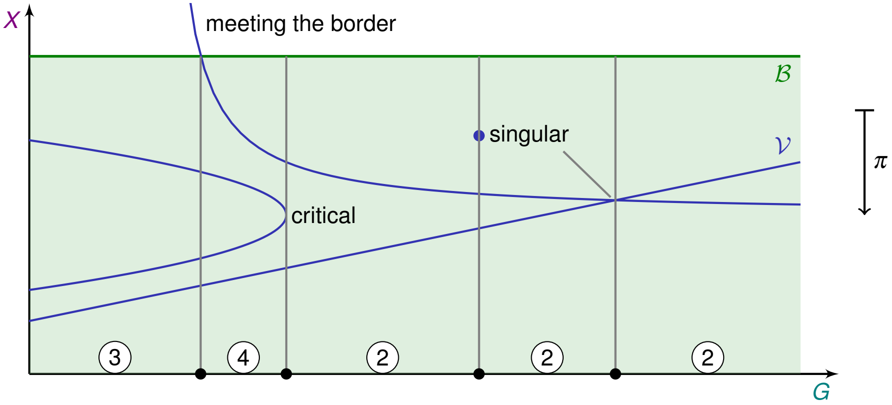

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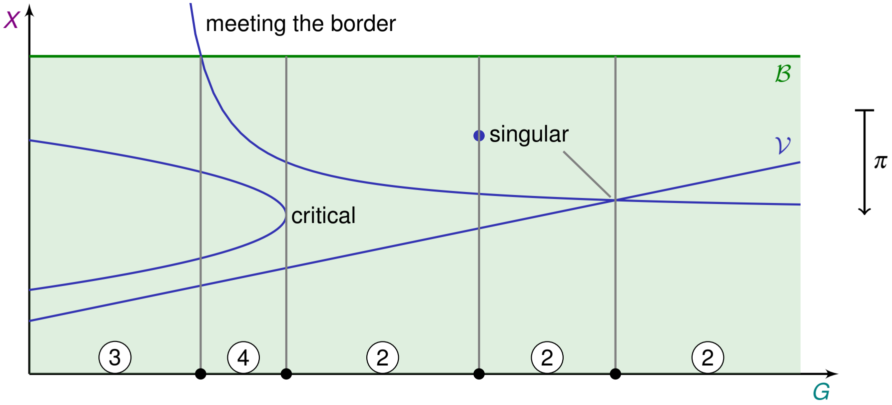

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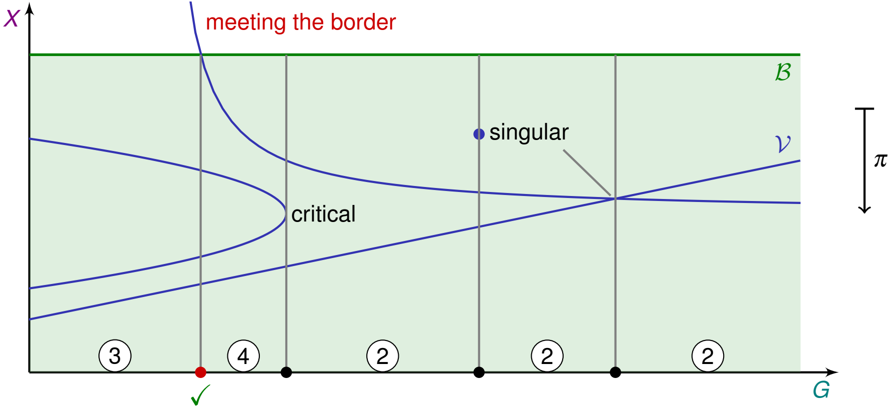
$\Big\} =: K(\pi, \mathcal{V})$

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

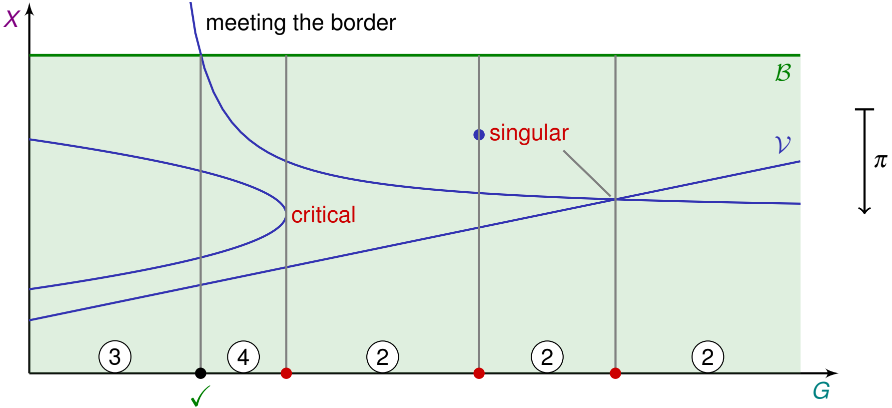
General strategy for the real roots classification problem



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**)



Critical and singular points

$$(\mathbf{X}, \mathbf{G}) \in K(\pi, \mathcal{V})$$
$$\iff \text{Jac}(F, \mathbf{X}) \text{ has rank } < d$$

Requirements

- F generates the ideal of $\mathcal{V}$ $\implies$ radical
- $\mathcal{V}$ is equidimensional with codimension d

Properties of determinantal systems

Determinantal systems

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

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For a generic matrix A with the same parameters

- $V_{\leq r}(A)$ equidimensional with codimension $(k - r)^2$
- $\text{Sing}(V_{\leq r}(A)) = V_{\leq r-1}(A)$, t-equidimensional
- $\text{Crit}(\pi, V_{\leq r}(A))$ 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)
- $V_{\leq r-1}(M)$ is equidimensional with dimension t
- $\mathcal{V} \setminus V_{\leq r-1}(M)$ has dimension $< t$
- Rank stratification : $\mathcal{V} = (\mathcal{V} \cap V_{\leq r-1}(M)) \cup (\mathcal{V} \setminus V_{\leq r-1}(M))$

Rank stratification

$$\mathcal{V} = K(\pi, V_{\leq r}(M))$$

$$\downarrow$$

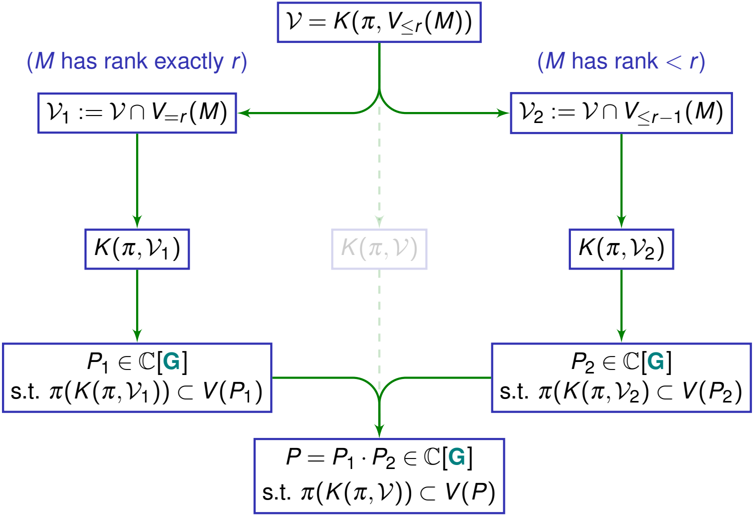
$$K(\pi, \mathcal{V})$$

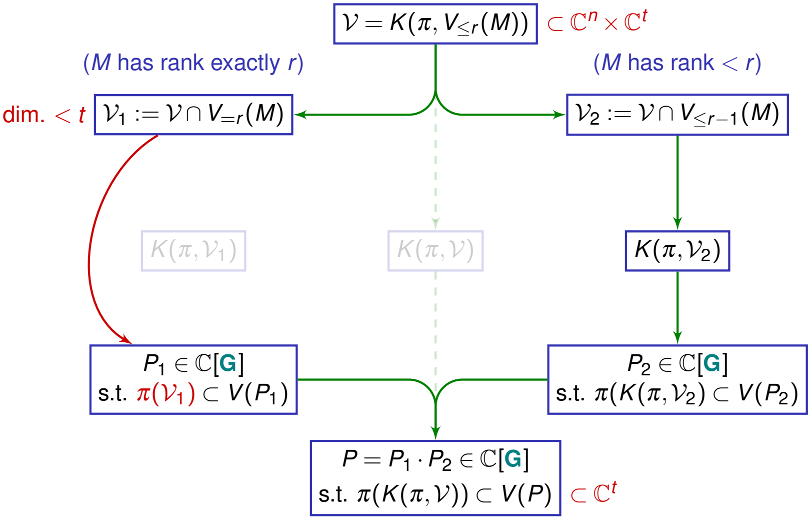
$$\downarrow$$

$$P \in \mathbb{C}[\mathbf{G}]$$

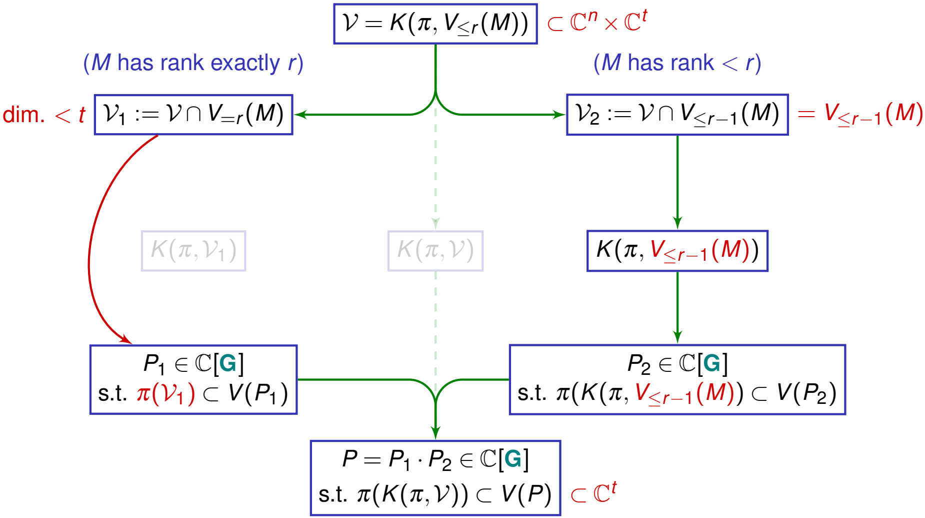
s.t. $\pi(K(\pi, \mathcal{V})) \subset V(P)$

Rank stratification




$\mathcal{V} = K(\pi, V_{\leq r}(M))$
$\subset \mathbb{C}^n \times \mathbb{C}^t$
(M has rank exactly r)
(M has rank $< r$)
dim. $< t$
$\mathcal{V}_1 := \mathcal{V} \cap V_{=r}(M)$
$\mathcal{V}_2 := \mathcal{V} \cap V_{\leq r-1}(M)$
$K(\pi, \mathcal{V}_1)$
$K(\pi, \mathcal{V})$
$K(\pi, \mathcal{V}_2)$
$P_1 \in \mathbb{C}[\mathbf{G}]$
s.t. $\pi(\mathcal{V}_1) \subset V(P_1)$
$P_2 \in \mathbb{C}[\mathbf{G}]$
s.t. $\pi(K(\pi, \mathcal{V}_2) \subset V(P_2)$
$P = P_1 \cdot P_2 \in \mathbb{C}[\mathbf{G}]$
s.t. $\pi(K(\pi, \mathcal{V})) \subset V(P)$
$\subset \mathbb{C}^t$

Rank stratification



Modelization using incidence varieties

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

Possible modelizations for determinantal varieties

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

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

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

Consequence for the strategy

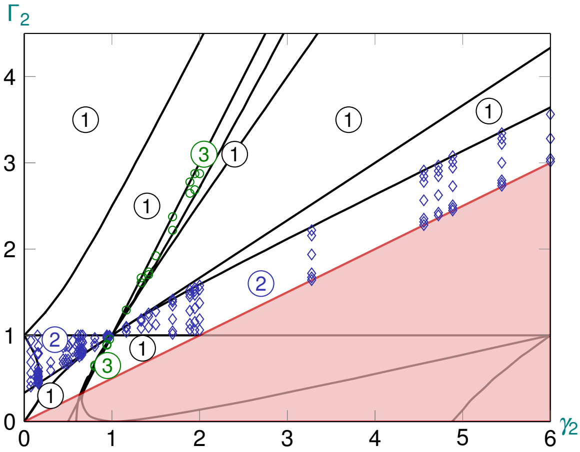
$K(\pi, V_{\leq r-1}(M))$ can be computed with the incidence system,
using maximal minors of the Jacobian matrix

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	46×200 s
Gröbner bases (`F5`)	-	1 s	-	110 s
Regular chains (`RegularChains`)	1050 s	-	$>$24 h	90×200 s

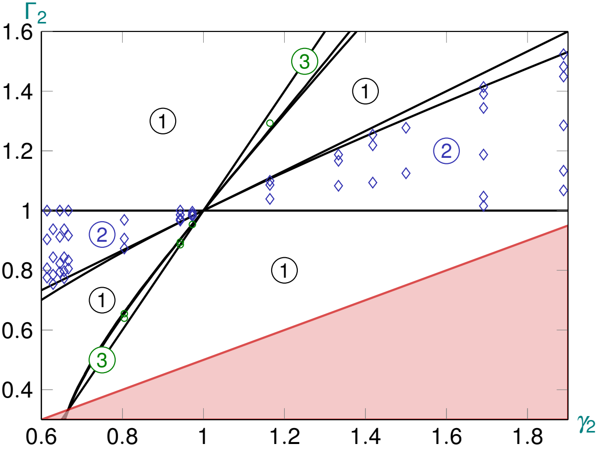
Results for the contrast problem in the case of water



Finishing the computations:

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

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



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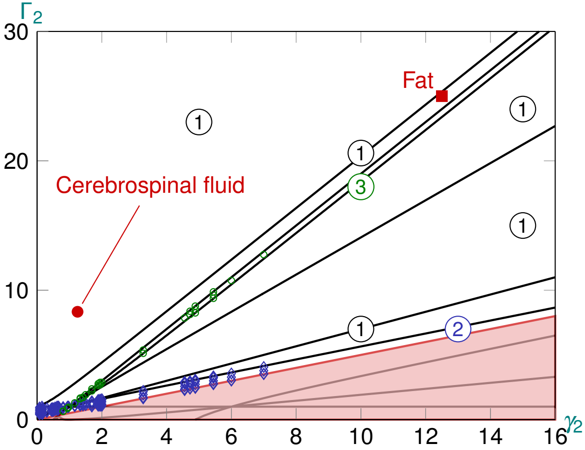

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Conclusion and perspectives

This work

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

Perspectives regarding the algorithms

Extensions to other structures:

- Incidence varieties for rectangular matrices
- Non-transverse intersection of determinantal varieties

And back to the dynamical problem

- Direct relation between the invariants and properties of the trajectories?
- Is it possible to lift some approximations?
- Further studies, for example cartography of the best possible contrast (LMI methods)

Thank you for your attention!

Results published in:

- B. Bonnard, J.-C. Faugère, A. Jacquemard, M. Safey El Din, T. 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