Determinantal sets, singularities and application to optimal control in medical imagery

Bernard Bonnard^{1,3} Jean-Charles Faugère² Alain Jacquemard^{1,2} Mohab Safey El Din² Thibaut Verron²

¹Institut de Mathématiques de Bourgogne, Dijon, France, UMR CNRS 5584

²Sorbonne Universités, UPMC Univ Paris 06, CNRS, Inria Paris, PolSys team

³Inria Sophia-Antipolis, McTao project

ISSAC'16, 20 July 2016

Physical problem

(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



Bad contrast (no enhancement)



Good contrast (enhanced)

Physical problem

(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



Bad contrast (no enhancement)



Good contrast (enhanced)

Known methods:

- inject contrast agents to the patient: potentially toxic
- make the field variable to exploit differences in relaxation times
 - \Rightarrow requires finding optimal settings depending on the relaxation parameters

Physical problem

(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



Bad contrast (no enhancement)

Examples of relaxation parameters:

- Water: $\gamma = \Gamma = 0.01 \text{ Hz}$
- Cerebrospinal fluid: $\gamma = 0.02 \text{ Hz}, \Gamma = 0.10 \text{ Hz}$
- Fat: $\gamma = 0.15 \,\text{Hz}, \Gamma = 0.31 \,\text{Hz}$



Good contrast (enhanced)

Numerical approach and computational problem

The Bloch equations

$$\begin{cases} \dot{y}_i &= -\Gamma_i y_i - \mathbf{u} z_i \\ \dot{z}_i &= -\gamma_i (1 - z_i) + \mathbf{u} y \end{cases}$$

(i = 1, 2)

Saturation method

Find a path u so that after some time T:

- matter 1 saturated: $y_1(T) = z_1(T) = 0$
- matter 2 "maximized": $|(y_2(T), z_2(T))|$ maximal

Glaser's team, 2012 : method from Optimal Control Theory

Numerical approach and computational problem

The Bloch equations

 $\begin{cases} \dot{y}_i &= -\Gamma_i y_i - u z_i \\ \dot{z}_i &= -\gamma_i (1 - z_i) + u y_i \end{cases}$

(i = 1, 2)

Saturation method

Find a path u so that after some time T:

- matter 1 saturated: $y_1(T) = z_1(T) = 0$
- matter 2 "maximized": $|(y_2(T), z_2(T))|$ maximal

Glaser's team, 2012 : method from Optimal Control Theory

Problem: analyze the behavior of the control through algebraic invariants

- Example: singular feedback control: $u = \frac{D'}{D} (D, D' \text{ polynomials in } y, z, \gamma, \Gamma)$
- Geometry of $\{D = 0\}$?
- Study of the singular points of $\{D = 0\}$ for each value of $\gamma_1, \Gamma_1, \gamma_2, \Gamma_2$
- Examples with water: [Bonnard, Chyba, Jacquemard, Marriott, 2013]
 - Water/Fat : 1 point

Water/Cerebrospinal fluid : 1 point

Numerical approach and computational problem

The Bloch equations

 $\begin{cases} \dot{y}_i &= -\Gamma_i y_i - u z_i \\ \dot{z}_i &= -\gamma_i (1 - z_i) + u y_i \end{cases}$

(*i* = 1, 2)

Saturation method

Find a path u so that after some time T:

- matter 1 saturated: $y_1(T) = z_1(T) = 0$
- matter 2 "maximized": $|(y_2(T), z_2(T))|$ maximal

Glaser's team, 2012 : method from Optimal Control Theory

Problem: analyze the behavior of the control through algebraic invariants

- Example: singular feedback control: $u = \frac{D'}{D} (D, D' \text{ polynomials in } y, z, \gamma, \Gamma)$
- Geometry of $\{D = 0\}$?
- Study of the singular points of $\{D = 0\}$ for each value of $\gamma_1, \Gamma_1, \gamma_2, \Gamma_2$
- Examples with water: [Bonnard, Chyba, Jacquemard, Marriott, 2013]
 - Water/Fat : 1 point
- Water/Cerebrospinal fluid : 1 point

Questions

- Is there always 1 singular point for pairs involving water?
- If not, how many possible families of parameters can we separate?

Statement of the semi-algebraic problem

The D invariant: equations of a determinantal system

$$M := \begin{cases} -\Gamma_1 y_1 & -z_1 - 1 & -\Gamma_1 + (\gamma_1 - \Gamma_1) z_1 & (2\gamma_1 - 2\Gamma_1) y_1 \\ -\gamma_1 z_1 & y_1 & (\gamma_1 - \Gamma_1) y_1 & 2\Gamma_1 - \gamma_1 - (2\gamma_1 - 2\Gamma_1) z_1 \\ -\Gamma_2 y_2 & -z_2 - 1 & -\Gamma_2 + (\gamma_2 - \Gamma_2) z_2 & (2\gamma_2 - 2\Gamma_2) y_2 \\ -\gamma_2 z_2 & y_2 & (\gamma_2 - \Gamma_2) y_2 & 2\Gamma_2 - \gamma_2 - (2\gamma_2 - 2\Gamma_2) z_2 \end{cases}$$

$$D := \text{determinant}(M)$$

$$V := \left\{ D = \frac{\partial D}{\partial y_1} = \frac{\partial D}{\partial z_1} = \frac{\partial D}{\partial y_2} = \frac{\partial D}{\partial z_2} = 0 \right\}$$

The Bloch ball: inequalities

►
$$B := \begin{cases} y_1^2 + (z_1 + 1)^2 \le 1 \\ y_2^2 + (z_2 + 1)^2 \le 1 \end{cases}$$

Goal

Classification of the real fibers of the projection of $V \cap B$ onto the parameter space

State of the art and contributions

State of the art:

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

State of the art and contributions

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?

State of the art and contributions

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?

Main results

- Dedicated strategy for real roots classification for determinantal systems
- Can use existing tools for elimination
- Main refinements:
 - Rank stratification
 - Incidence varieties

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?

Main results

- 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
 - Answers to the experimental questions for water: there can be 1, 2 or 3 singularities





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

▶ projections of points where *V* meets the border of the semi-algebraic domain



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

- projections of points where V meets the border of the semi-algebraic domain
- critical values of π_G restricted to V



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

- projections of points where V meets the border of the semi-algebraic domain
- critical values of π_G restricted to V
- projections of singular points of V



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

- ▶ projections of points where V meets the border of the semi-algebraic domain
- critical values of π_G restricted to V
- projections of singular points of V

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

How to compute these points

Goal: compute $P \in \mathbb{Q}[\gamma, \Gamma]$ such that

$$V(P) \supset \pi((V \cap \partial B) \cup \operatorname{Sing}(V) \cup \operatorname{Crit}(\pi, V))$$

with

•
$$\pi$$
: projection onto the parameters γ_i, Γ_i
• $V = \left\{ D = \frac{\partial D}{\partial y_1} = \frac{\partial D}{\partial z_1} = \frac{\partial D}{\partial y_2} = \frac{\partial D}{\partial z_2} = 0 \right\}$
• $B = \left\{ y_1^2 + (z_1 + 1)^2 \le 1, y_2^2 + (z_2 + 1)^2 \le 1 \right\}$

Intersection with the border

Compute:

- $V \cap \{y_1^2 + (z_1 + 1)^2 = 1\}$
- $V \cap \{y_2^2 + (z_2 + 1)^2 = 1\}$

and their image through π

(polynomial elimination)

How to compute these points

Goal: compute $P \in \mathbb{Q}[\gamma, \Gamma]$ such that

$$V(P) \supset \pi((V \cap \partial B) \cup \operatorname{Sing}(V) \cup \operatorname{Crit}(\pi, V))$$

with

•
$$\pi$$
: projection onto the parameters γ_i, Γ_i
• $V = \left\{ D = \frac{\partial D}{\partial y_1} = \frac{\partial D}{\partial z_1} = \frac{\partial D}{\partial y_2} = \frac{\partial D}{\partial z_2} = 0 \right\}$
• $B = \left\{ y_1^2 + (z_1 + 1)^2 \le 1, y_2^2 + (z_2 + 1)^2 \le 1 \right\}$

Intersection with the border

Compute:

- $V \cap \{y_1^2 + (z_1 + 1)^2 = 1\}$
- $V \cap \{y_2^2 + (z_2 + 1)^2 = 1\}$

and their image through π

(polynomial elimination)

Critical and singular points

$$(\mathbf{y}, \mathbf{z}, \gamma, \Gamma) \in \operatorname{Sing}(V) \cup \operatorname{Crit}(\pi, V)$$

 $\iff \operatorname{Jac}(F, (\mathbf{y}, \mathbf{z})) \text{ has rank } < d$

Requirements

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

- $A = k \times k$ -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: n = 4, k = 4, r = 3, $V = \text{Sing}_{y_1, y_2, z_1, z_2}(V_{\leq r}(M))$

- $A = k \times k$ -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: n = 4, k = 4, r = 3, $V = \text{Sing}_{y_1, y_2, z_1, z_2}(V_{\leq r}(M))$

With a generic matrix A

With our specific matrix M

$$\blacktriangleright V_{\leq r-1}(M) \subset V$$

• dim
$$(V) = t$$

$$\blacktriangleright \dim(V \smallsetminus V_{\leq r-1}) < t$$

• $V_{\leq r-1}(M)$ equidimensional

$$\blacktriangleright \dim(V_{\leq r-1}(M)) = t$$

• $\operatorname{Sing}_{\mathbf{X}}(V_{\leq r}(A)) = V_{\leq r-1}(A)$

V_{≤r}(A) equidimensional

• dim
$$(V_{\leq r}(A)) = n + t - (k - r)^2$$

 \implies dim $(V_{\leq r-1}(A)) = t$

- $A = k \times k$ -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:
$$n = 4$$
, $k = 4$, $r = 3$, $V = \text{Sing}_{y_1, y_2, z_1, z_2}(V_{\leq r}(M))$



- $A = k \times k$ -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:
$$n = 4$$
, $k = 4$, $r = 3$, $V = \text{Sing}_{y_1, y_2, z_1, z_2}(V_{\leq r}(M))$



Goal: $P \subset \mathbb{Q}[\gamma, \Gamma]$ such that $V(P) \supset \pi(\operatorname{Sing}(V) \cup \operatorname{Crit}(\pi, V))$ with $\pi : \mathbb{C}^{n+t} \to \mathbb{C}^{t}$

Rank stratification

$$V = (V \cap V_{=r}) \cup (V \cap V_{\leq r-1})$$

•
$$V \cap V_{=r}$$
: dimension $< t$

• $V \cap V_{\leq r-1} = V_{\leq r-1}$: *t*-equidimensional

Consequence for the strategy

- 1. Compute P_1 such that $V(P_1) \supset \pi(V \cap V_{=r})$
- 2. Compute P_2 such that $V(P_2) \supset \pi(\text{Sing}(V_{\leq r-1}(M)) \cup \text{Crit}(\pi, V_{\leq r-1}(M)))$
- 3. Return $P := P_1 \cdot P_2$

Goal: $P \subset \mathbb{Q}[\gamma, \Gamma]$ such that $V(P) \supset \pi(\operatorname{Sing}(V) \cup \operatorname{Crit}(\pi, V))$ with $\pi : \mathbb{C}^{n+t} \to \mathbb{C}^{t}$

Rank stratification

$$V = (V \cap V_{=r}) \cup (V \cap V_{\leq r-1})$$

•
$$V \cap V_{=r}$$
: dimension $< t$

• $V \cap V_{\leq r-1} = V_{\leq r-1}$: *t*-equidimensional

Consequence for the strategy

- 1. Compute P_1 such that $V(P_1) \supset \pi(V \cap V_{=r})$
- 2. Compute P_2 such that $V(P_2) \supset \pi(\text{Sing}(V_{\leq r-1}(M)) \cup \text{Crit}(\pi, V_{\leq r-1}(M)))$
- 3. Return $P := P_1 \cdot P_2$

Change of model: 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) $\leq r \iff \exists L, A \cdot L = 0$ 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
- Codimension: $(k-r)^2 + k(k-r)$

Change of model: 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) $\leq r \iff \exists L, A \cdot L = 0$ 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
- Codimension: $(k-r)^2 + k(k-r)$

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

- It defines a radical ideal
- It forms a regular sequence (codimension = length)
 - \implies Critical points characterized by maximal minors of the Jacobian matrix

Consequence for the strategy

Sing($V_{\leq r-1}(M)$) \cup Crit(π , $V_{\leq r-1}(M)$) can be computed with the incidence system



Answers to the questions

- There can be 1, 2 or 3 singular points in the fibers
- We can separate 3 families of biological matters

Results for water (zoom in)



Answers to the questions

- There can be 1, 2 or 3 singular points in the fibers
- We can separate 3 families of biological matters

Results for water (zoom out)



Answers to the questions

- There can be 1, 2 or 3 singular points in the fibers
- We can separate 3 families of biological matters

Timings

- 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	$90 \times 200\text{s}$

What has been done?

- Algorithmic strategy for real roots classification with determinantal varieties
- Exploiting the determinantal structure
- Successfully applied in an application to contrast optimization in MRI

The future

- Complexity bounds
- Contrast optimization: other criteria of the classification still need to be studied
- New numerical questions about small areas in the classification

What has been done?

- Algorithmic strategy for real roots classification with determinantal varieties
- Exploiting the determinantal structure
- Successfully applied in an application to contrast optimization in MRI

The future

- Complexity bounds
- Contrast optimization: other criteria of the classification still need to be studied
- New numerical questions about small areas in the classification

Thank you!