# Algebraic classification related to contrast optimization for MRI 

Bernard Bonnard ${ }^{1}$ Jean-Charles Faugère ${ }^{2}$
Alain Jacquemard ${ }^{1,2}$ Mohab Safey El Din ${ }^{2}$ Thibaut Verron ${ }^{2}$

```
'1 Institut de Mathématiques de Bourgogne, Dijon, France
                        UMR CNRS 5584
\({ }^{2}\) Université Pierre et Marie Curie, Paris 6, France INRIA Paris-Rocquencourt, Équipe PoLSYs
Laboratoire d'Informatique de Paris 6, UMR CNRS 7606
```

Journées du GdR MOA, 3 décembre 2015

## Physical problem

(N)MRI = (Nuclear) Magnetic Resonance Imagery

1. apply a magnetic field to a body
2. measure the radio waves emitted in reaction

Optimize the contrast = be able to distinguish two biological matters from this measure


Bad contrast (no enhancement)

Known methods:

- inject contrast agents to the patient: potentially toxic
- make the field variable to exploit differences in relaxation times
$\Longrightarrow$ 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

Optimize the contrast = be able to distinguish two biological matters from this measure


Examples:

- Bio. matter 1: Deoxygenated blood ( $\gamma_{1} \simeq 0.74 \mathrm{~Hz}, \Gamma_{1}=20 \mathrm{~Hz}$ )
- Bio. matter 2: Oxygenated blood ( $\gamma_{2}=0.74 \mathrm{~Hz}, \Gamma_{2} \simeq 5 \mathrm{~Hz}$ )


## Physical problem

(N)MRI = (Nuclear) Magnetic Resonance Imagery

1. apply a magnetic field to a body
2. measure the radio waves emitted in reaction

Optimize the contrast = be able to distinguish two biological matters from this measure


Examples:

- Bio. matter 1: Water ( $\gamma_{1}=\Gamma_{1}=0.4 \mathrm{~Hz}$ )
- Bio. matter 2: Cerebrospinal fluid ( $\gamma_{2}=0.5 \mathrm{~Hz}, \Gamma_{2} \simeq 3.3 \mathrm{~Hz}$ )


## Numerical approach

## The Bloch equations

$\left\{\begin{array}{l}\dot{y}_{i}=-\Gamma_{i} y_{i}-u \cdot z_{i} \\ \dot{z}_{i}=-\gamma_{i}\left(1-z_{i}\right)+u \cdot y_{i}\end{array}(i=1,2)\right.$
Bonnard, Glaser : Control Theory problem

## Saturation method

Find a path $t \mapsto u(t)$ so that after some time $T$ :

- matter 1 saturated: $y_{1}(T)=z_{1}(T)=0$
- matter 2 "maximized": $\left|\left(y_{2}(T), z_{2}(T)\right)\right|$ maximal



## Problem (Bonnard et al. 2013)

- The length $T$ of the path is not bounded
- Goal: better understand the control problem to obtain optimal solutions
- Classify invariants of a related differential equation


## The invariants $D$ and $D^{\prime}$

## Expression for $D$ ( $D^{\prime}$ has an analogous definition)

- $\boldsymbol{M}:=\left(\begin{array}{cccc}-\Gamma_{1} y_{1} & -z_{1}-1 & -\Gamma_{1}+\left(\gamma_{1}-\Gamma_{1}\right) z_{1} & \left(2 \gamma_{1}-2 \Gamma_{1}\right) y_{1} \\ -\gamma_{1} z_{1} & y_{1} & \left(\gamma_{1}-\Gamma_{1}\right) y_{1} & 2 \Gamma_{1}-\gamma_{1}-\left(2 \gamma_{1}-2 \Gamma_{1}\right) z_{1} \\ -\Gamma_{2} y_{2} & -z_{2}-1 & -\Gamma_{2}+\left(\gamma_{2}-\Gamma_{2}\right) z_{2} & \left(2 \gamma_{2}-2 \Gamma_{2}\right) y_{2} \\ -\gamma_{2} z_{2} & y_{2} & \left(\gamma_{2}-\Gamma_{2}\right) y_{2} & 2 \Gamma_{2}-\gamma_{2}-\left(2 \gamma_{2}-2 \Gamma_{2}\right) z_{2}\end{array}\right)$
- $D:=\operatorname{det}(M)$


## Properties:

- Homogeneous in the parameters $\gamma_{i}, \Gamma_{i}$, degree 3
- Degree 4 in the variables $y_{i}, z_{i}$

Now the problem is algebraic!

## Goal

Classification of the invariants in terms of $\Gamma_{i}, \gamma_{i}$ :

- Singularities of $\{D=0\}$
- Surface $\left\{D=D^{\prime}=0\right\}$
- Curve of singularities of $\left\{D=D^{\prime}=0\right\}$


## The invariants $D$ and $D^{\prime}$

Expression for $D$ ( $D^{\prime}$ has an analogous definition)

- $M:=\left(\begin{array}{cccc}-\Gamma_{1} y_{1} & -z_{1}-1 & -\Gamma_{1}+\left(\gamma_{1}-\Gamma_{1}\right) z_{1} & \left(2 \gamma_{1}-2 \Gamma_{1}\right) y_{1} \\ -\gamma_{1} z_{1} & y_{1} & \left(\gamma_{1}-\Gamma_{1}\right) y_{1} & 2 \Gamma_{1}-\gamma_{1}-\left(2 \gamma_{1}-2 \Gamma_{1}\right) z_{1} \\ -\Gamma_{2} y_{2} & -z_{2}-1 & -\Gamma_{2}+\left(\gamma_{2}-\Gamma_{2}\right) z_{2} & \left(2 \gamma_{2}-2 \Gamma_{2}\right) y_{2} \\ -\gamma_{2} z_{2} & y_{2} & \left(\gamma_{2}-\Gamma_{2}\right) y_{2} & 2 \Gamma_{2}-\gamma_{2}-\left(2 \gamma_{2}-2 \Gamma_{2}\right) z_{2}\end{array}\right)$
- $D:=\operatorname{det}(M)$

Properties:

- Homogeneous in the parameters $\gamma_{i}, \Gamma_{i}$, degree 3
- Degree 4 in the variables $y_{i}, z_{i}$

Now the problem is algebraic!

## Goal

Classification of the invariants in terms of $\Gamma_{i}, \gamma_{i}$ :

- Singularities of $\{D=0\}$
- Surface $\left\{D=D^{\prime}=0\right\}$
- Curve of singularities of $\left\{D=D^{\prime}=0\right\}$


## Overview of the results: singularities of $\{D=0\}$ in terms of $\Gamma_{i}, \gamma_{i}$

Singularities are invariant under $\left(y_{i} \mapsto-y_{i}\right)$


Classification in terms of $\Gamma_{i}, \gamma_{i}$ :

- Generically: 4 pairs of singularities for each value of the parameters
- 3 pairs for each value on a surface with 5 components
- one hyperplane
- one quadric
- one quartic
- one degree 14 surface
> onie degree 24 surface
- 2 pairs for each value on a curve with many components
- 1 pair for each value on a set of
points.


## Overview of the results: singularities of $\{D=0\}$ in terms of $\Gamma_{i}, \gamma_{i}$

Singularities are invariant under ( $y_{i} \mapsto-y_{i}$ )


Classification in terms of $\Gamma_{i}, \gamma_{i}$ :

- Generically: 4 pairs of singularities for each value of the parameters
- 3 pairs for each value on a surface with 5 components
- one hyperplane
- one quadric
- one quartic
- one degree 14 surface
- one degree 24 surface
- 2 pairs for each value on a curve with many components
- 1 nair for each value on a set of points.

Overview of the results: singularities of $\{D=0\}$ in terms of $\Gamma_{i}, \gamma_{i}$

Singularities are invariant under $\left(y_{i} \mapsto-y_{i}\right)$


Classification in terms of $\Gamma_{i}, \gamma_{i}$ :

- Generically: 4 pairs of singularities for each value of the parameters
- 3 pairs for each value on a surface with 5 components
- one quadric
- one quartic 14 surface
- one degree 24 surface
- 2 pairs for each value on a curve with many components
- 1 pair for each value on a set of

Overview of the results: singularities of $\{D=0\}$ in terms of $\Gamma_{i}, \gamma_{i}$

Singularities are invariant under $\left(y_{i} \mapsto-y_{i}\right)$


Classification in terms of $\Gamma_{i}, \gamma_{i}$ :

- Generically: 4 pairs of singularities for each value of the parameters
- 3 pairs for each value on a surface with 5 components
- one quadric
- one quartic
- one degree 14 surface
- one degree 24 surface
- 2 pairs for each value on a curve with many components
- 1 pair for each value on a set of
points


## Overview of the results: singularities of $\{D=0\}$ in terms of $\Gamma_{i}, \gamma_{i}$

Singularities are invariant under ( $y_{i} \mapsto-y_{i}$ )


Classification in terms of $\Gamma_{i}, \gamma_{i}$ :

- Generically: 4 pairs of singularities for each value of the parameters
- 3 pairs for each value on a surface with 5 components
- one quadric
- one quartic 14 surface
- one degree 24 surface
- 2 pairs for each value on a curve with many components
- 1 pair for each value on a set of points...


## Tool: Gröbner bases

## What is it?

- Tool for solving polynomial systems
- If finite number of (complex) solutions: enumerations of the solutions as:

$$
\left\{\begin{array}{l}
P_{1}\left(X_{1}\right)=0 \\
X_{i}-P_{i}\left(X_{1}\right)=0
\end{array}\right.
$$

- For systems with positive dimension: allows to compute projections
- Known since the 60s, now available in most computer algebra software


## Advantages

- Exact computations: no solutions are left out
- Able to take advantage of algebraic or geometric structures
- More equations is usually better!


## Caveats

- Long computations, complexity not known beforehand
- Complicated results (high degree, large polynomials)
- Global method: we can only localise on dense subsets


## How do we use Gröbner bases on this problem?

## Key idea: importance of the modelization

- The complexity depends on the system, rather than on its solutions
- Idea: choose a particular system with nicer properties
- Examples: lower degree, less indeterminates, more equations...
- Usually, it means a tradeoff!


## State of the art for the current problem

- General case $\longrightarrow 4$ variables, 4 parameters
- Particular cases $\longrightarrow 0$ parameters

Intractable
(Bonnard et al. 2013)

## Application to the current problem

Filling the gap between the two extremes above

- Simplification by homogeneity $\gamma_{1}=1 \longrightarrow 3$ parameters

Intractable

- Intermediate cases (e.g. water: $\gamma_{1}=\Gamma_{1}=1$ ) $\longrightarrow 2$ parameters

Attacking the general classification: decompositions into subproblems

## Example of decomposition: rank of the matrix

We split the problem depending on the rank of the matrix:

$$
\operatorname{det}(M)=0 \Longrightarrow\left\{\begin{array}{c}
\operatorname{rank}(M)=3 \\
\operatorname{or} \\
\operatorname{rank}(M)<3
\end{array}\right.
$$

Why the rank? Because of...

## Theorem

Consider

$$
M=\left(P_{i, j}(\mathbf{X})\right)_{1 \leq i, j \leq n}
$$

Then generically:

$$
\operatorname{det}(M) \text { singular } \Longrightarrow \operatorname{rank}(M)<n-1
$$

With this specific matrix, the theorem does not apply.
$\Longrightarrow$ There are solutions in both branches.

| Case | Solutions in $\Gamma_{1}, \Gamma_{2}, \gamma_{2}$ |
| ---: | :--- |
| $\operatorname{rank}(M)<3$ | Dimension 3 |
| $\operatorname{rank}(M)=3$ | Dimension 2 |

## Classification in the generic case $\operatorname{rank}(M)<3$

We append all $3 \times 3$ minors of $M$ to the system
(Remember: more equations is better!)
Through a (long) Gröbner basis computation, we can find in the ideal:

$$
P=\sum_{d=0}^{4} a_{d}\left(\Gamma_{1}, \Gamma_{2}, \gamma_{2}\right) y_{2}{ }^{2 d}
$$

It is a large polynomial (1776 monomials...) but with a nice structure:

- Degree 4 in $y_{2}^{2}$
- Non-irreducible coefficients in $y_{2}$, high degree common factors


## Classification: number of roots of $P\left(y_{2}\right)$

- Generically: 4 pairs of opposite solutions
- If $a_{4}=0$ or $\operatorname{disc}(P)=0$, generically: 3 pairs of solutions
- 3 components from the factorization of $a_{4}$
- 2 components from the factorization of $\operatorname{disc}(P)$



## Example of change of model: what to do if $\operatorname{rank}(M)=3$ ?

## Theorem

Consider $M=\left(P_{i, j}(\mathbf{X})\right)_{1 \leq i, j \leq n}$ and let $\mathcal{I}$ be the incidence variety defined by

$$
\left[\begin{array}{l}
M
\end{array}\right] \cdot\left[\begin{array}{c}
\lambda_{1} \\
\vdots \\
\lambda_{n}
\end{array}\right]=\left[\begin{array}{c}
0 \\
\vdots \\
0
\end{array}\right]
$$

If $(\mathbf{x})$ is a point of $\{\operatorname{det}(M(\mathbf{x}))=0\}$, then:

- there exists a non-zero vector $\Lambda=\left(\lambda_{i}\right)$ such that $(\mathbf{x}, \Lambda) \in \mathcal{I}$


## Example of change of model: what to do if $\operatorname{rank}(M)=3$ ?

## Theorem

Consider $M=\left(P_{i, j}(\mathbf{X})\right)_{1 \leq i, j \leq n}$ and let $\mathcal{I}$ be the incidence variety defined by

$$
\left[\begin{array}{l} 
\\
M
\end{array}\right] \cdot\left[\begin{array}{c}
\lambda_{1} \\
\vdots \\
\lambda_{n}
\end{array}\right]=\left[\begin{array}{c}
0 \\
\vdots \\
0
\end{array}\right]
$$

If $(\mathbf{x})$ is a singular point of $\{\operatorname{det}(M(\mathbf{x}))=0\}$ such that $M(\mathbf{x})$ has rank $n-1$, then:

- there exists a non-zero vector $\Lambda=\left(\lambda_{i}\right)$ such that $(\mathbf{x}, \Lambda) \in \mathcal{I}$, and
- $\wedge$ is unique up to scalar multiplication, and
- $(\mathbf{x}, \Lambda)$ is a singular point of $\mathcal{I}$ w.r.t. $\mathbf{X}$


## Example of change of model: what to do if $\operatorname{rank}(M)=3$ ?

## Theorem

Consider $M=\left(P_{i, j}(\mathbf{X})\right)_{1 \leq i, j \leq n}$ and let $\mathcal{I}$ be the incidence variety defined by

$$
\left[\begin{array}{l}
M
\end{array}\right] \cdot\left[\begin{array}{c}
\lambda_{1} \\
\vdots \\
\lambda_{n}
\end{array}\right]=\left[\begin{array}{l}
0 \\
\vdots \\
0
\end{array}\right]
$$

If $(\mathbf{x})$ is a singular point of $\{\operatorname{det}(M(\mathbf{x}))=0\}$ such that $M(\mathbf{x})$ has rank $n-1$, then:

- there exists a non-zero vector $\Lambda=\left(\lambda_{i}\right)$ such that $(\mathbf{x}, \Lambda) \in \mathcal{I}$, and
- $\Lambda$ is unique up to scalar multiplication, and
- $(\mathbf{x}, \Lambda)$ is a singular point of $\mathcal{I}$ w.r.t. $\mathbf{X}$

$$
\begin{aligned}
& \langle D, \frac{\partial D}{\partial y_{i}}, \frac{\partial D}{\partial z_{i}}, \underbrace{M \cdot \Lambda, \operatorname{rank}\left(\nabla_{y_{i}, z_{i}}(M \cdot \Lambda)<4\right)}_{\Lambda}, \underbrace{\mathcal{M}_{k} \neq 0}_{\Lambda}, \underbrace{\substack{1 \leq k \leq 16 \\
1 \leq i \leq 4}}_{\substack{\lambda_{i}=1}} \\
& \text { Singular point of } \\
& \text { the incidence variety } \\
& \text { Non-zero } \\
& 3 \times 3 \text { minor } \\
& \text { (16 choices) }
\end{aligned}
$$

## Conclusion and perspectives

## What has been done?

Part of the classification of invariants for the saturation problem

- Exhaustive classification in some particular cases (water)
- Some branches entirely explored in full generality


## Still work in progress

- Some branches not solved yet in full generality
- Some parameters of the classification still need to be studied ( $D^{\prime}$ )


## Applications

- New control policies for contrast optimisation for the MRI
- More generally, computational strategy applicable to similar problems


## One last word



Thank you for your attention! Merci pour votre attention!

