Régularisation du calcul de bases de Gröbner pour des systèmes avec poids et déterminantiels, et application en imagerie médicale

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## An example: the contrast optimisation problem (1)

(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 (not enhanced)



Good contrast (enhanced)

#### Known methods:

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

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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)

## An example: the contrast optimization problem (2)

The Bloch equations

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



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Problem: analyze the behavior of the control through algebraic invariants

- ► Example: singular feedback control:  $u = \frac{D'}{D}$  (*D*, *D'* polynomials in *y*,*z*,*γ*, $\Gamma$ )
- ▶ 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

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### Questions

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

### An example: the polynomial system

#### The D invariant: equation of a determinantal system

• 4 variables ( $y_i, z_i, i = 1, 2$ ) and 4 parameters ( $\gamma_i, \Gamma_i, i = 1, 2$ )

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

► D := determinant(M)

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

### Polynomial system with structure

- 5 equations of degree 8 in 4 variables and 4 parameters
- Homogeneous in  $\gamma$ ,  $\Gamma$ , degree 4
- Roots of D = points where M has rank  $\leq$  3 : determinantal system
- V = singularities and critical points of the determinantal variety

## Polynomial system solving

#### Applications:

- Control theory
- Cryptography
- Physics, industry...

Polynomial equations  $f_1(\mathbf{X}) = \cdots = f_m(\mathbf{X}) = 0$ 

### Examples of solutions:

. . .

- Find all the solutions if finite (dimension 0)
- Eliminate some variables (dimension > 0)

- Numerical: give approximations of the solutions
  - Newton's method
  - Homotopy continuation method
- Symbolic: give exact solutions
  - Gröbner bases
  - Resultant method
  - Triangular sets
  - Geometric resolution

### Difficult problem

- Exponential number of solutions
- NP-complete (at least on finite fields)

### What is the goal for the contrast optimization example?

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The Bloch ball: inequalities ~> real semi-algebraic set

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$$\mathcal{B} := \left\{ \begin{array}{c} y_1^2 + (z_1 + 1)^2 \leq 1 \\ y_2^2 + (z_2 + 1)^2 \leq 1 \end{array} \right\}$$

### Goal

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





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- Projections ( \leftarrow elimination)
- Critical and singular points

## Algebraic regularity

### How to compute singular and critical points?

- Definition depends on the dimension of irreducible components
- Can be characterized globally using the rank of a truncated Jacobian matrix for equidimensional varieties

#### Definition

$$\begin{split} \mathbf{F} &= (f_1, \dots, f_m) \in \mathbb{K}[\mathbf{X}] \text{ is regular iff} \\ \begin{cases} \langle F \rangle \subsetneq \mathbb{K}[\mathbf{X}] \\ \forall i, f_i \text{ is no zero-divisor in } \mathbb{K}[\mathbf{X}] / \langle f_1, \dots, f_{i-1} \rangle \end{cases} \end{split}$$



### **Properties**

- F regular  $\iff V(F)$  equidimensional with dimension n-m
- Regular sequences are generic (amongst systems of polynomials with given degrees)

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#### Degree 10 Regular Gröbner basis algorithms (e.g. F<sub>5</sub>) Irregular Compute a basis by iteratively 8 building and reducing matrices of polynomials of same degree 6 Normal strategy: perform lowest-degree reductions first Degree falls 4 Degree = indicator of progress Step

0

2

6

4

8

10

12

#### Degree fall?

- Definition: reduction resulting in a lower degree polynomial
- Example:  $X \cdot (Y-1) Y \cdot (X-1) = XY YX + Y X$
- ► Consequence: "next d" < d+1</p>



#### Regular sequences $\implies$ algorithmic regularity!

- ▶  $F_5$ -criterion: no reduction to zero in  $F_5$  (  $\iff$  all matrices have full-rank)
- ► Degree falls ⇐⇒ Reduction to zero of the highest degree components

→ Regularity in the affine sense = regularity of the highest degree components



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This notion depends on the homogeneous structure!

### Complexity for generic homogeneous systems if n = m



## Context and main results



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### Why the weights? An example (1)

Discrete Logarithm Problem on Edwards elliptic curves (Faugère, Gaudry, Huot, Renault 2013)



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## Why the weights? An example (3)

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Alt. strategy: use weights

= substitute  $X_i \leftarrow X_i^{w_i}$  for  $W = (w_1, \ldots, w_5)$ 

What weights?

- ► W = (1,1,1,1,1): nothing changed
- ▶ *W* = (2,2,1,1,1): better...
- W = (2, 2, 2, 2, 1): regular!

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System of weights:  $W = (w_1, \ldots, w_n) \in \mathbb{N}^n$ 

Weighted degree (or *W*-degree):  $\deg_W(X_1^{\alpha_1} \dots X_n^{\alpha_n}) = \sum_{i=1}^n w_i \alpha_i$ 

Weighted homogeneous polynomial: poly. containing only monomials of same W-degree

 $\rightarrow$  Example: physical equations: Volume=Area  $\times$  Height

Given a general (non-weighted-homogeneous) system and a system of weights

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### Strategy and complexity for W-homogeneous systems



### Why is the strategy correct?



# Why is the strategy correct?



# Regularity: homogeneous vs W-homogeneous

Properties of regular sequences				
	Homogeneous	W-homogeneous		
F <sub>5</sub> Criterion?	Yes	Yes		
Generic?	Yes	$lf \neq \varnothing$		
Bézout's bound	$\deg(\langle F\rangle) = \prod_{i=1}^n d_i$	$deg(\langle F  angle) = rac{\prod_{i=1}^n d_i}{\prod_{i=1}^n w_i}$		
Macaulay's bound	$d_{\max} \leq \sum_{i=1}^n (d_i - 1) + 1$	$d_{\max} \leq \sum_{i=1}^n (d_i - w_i) + \max\{w_j\}$		
Macaulay's bound reached?	Yes	Not always		

Macaulay's bound requires to know how each variable participates in the computations

### Simultaneous Noether position

- " $f_1, \ldots, f_i$  depend on  $X_1, \ldots, X_i$ " for all i
- SNP is "as generic as possible" too
- Weighted Macaulay's bound if in SNP:  $d_{max} \leq \sum_{i=1}^{n} (d_i w_i) + w_n$

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Two-step strategy for 0-dimensional systems

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System	Normal (s)	Weighted (s)	Speed-up
DLP Edwards $n = 5$ , GREvLEX (F <sub>5</sub> , FGb)	6461.2	935.4	6.9
DLP Edwards $n = 5$ , GREvLEX (F <sub>4</sub> , Magma)	56195.0	6044.0	9.3
Invariant relations, Cyclic $n = 5$ , GREvLEX (F <sub>4</sub> , Magma)	>75000	392.7	>191
Monomial relations, $n = 26$ , $m = 52$ , GREVLEX (F <sub>4</sub> , Magma)	14630.6	0.2	73153
DLP Edwards $n = 5$ , LEX (Sparse-FGLM, FGb)	6835.6	2164.4	3.2
Invariant relations, Cyclic $n = 5$ , ELIM (F <sub>4</sub> , Magma)	NA	382.5	NA
Monomial relations, $n = 26$ , $m = 52$ , ELIM (F <sub>4</sub> , Magma)	17599.5	8054.2	2.2

### Singularities of determinantal systems



# Setting for the contrast optimization problem

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

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- Dedicated strategy for real roots classification for determinantal systems
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- Main refinements:
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#### 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



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singular points of 
$${\cal V}$$

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

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  $\pi$  (eliminate X)



Can we find a regular sequence for F?

#### Determinantal systems

- $A = k \times k$ -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:  $n = 4, k = 4, r = 3, V = K(\pi, V_{\leq r}(M))$ 

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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
- $\operatorname{Crit}(\pi, V_{\leq r}(A))$  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 :  $\mathcal{V} = (\mathcal{V} \cap V_{\leq r-1}(M)) \cup (\mathcal{V} \setminus V_{\leq r-1}(M))$









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

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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

### Experimental results: 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	$90 \times 200\text{s}$
#### Experimental results: answers



#### Answers to the questions

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



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# Thank you for your attention!

Publications:

- Jean-Charles Faugère, Mohab Safey El Din and Thibaut Verron (2013). 'On the complexity of computing Gröbner bases for quasi-homogeneous systems'. In: Proceedings of the 2013 International Symposium on Symbolic and Algebraic Computation. ISSAC '13. Boston, USA: ACM
- Jean-Charles Faugère, Mohab Safey El Din and Thibaut Verron (2016). 'On the complexity of computing Gröbner bases for weighted homogeneous systems'. In: *Journal of Symbolic Computation* 76, pp. 107–141. ISSN: 0747-7171. DOI: http://dx.doi.org/10.1016/j.jsc.2015.12.001. URL: http://www.sciencedirect.com/science/article/pii/S0747717115001273
- Bernard Bonnard, Jean-Charles Faugère, Alain Jcquemard, 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