Algebraic issues in the contrast problem in Nuclear Magnetic Resonance.

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Part I

Nuclear Magnetic Resonance spectroscopy

informatiques mathématiques

Introduction

Main program: improve contrast in Nuclear Magnetic Resonance spectroscopy.

Joint project with Bernard Bonnard (INRIA, Dijon), Monique Chyba and John Marriott (Hawai), Mathieu Claeys (Cambridge, LAAS Toulouse), Olivier Cots (INRIA, Toulouse), Pierre Martinon (Polytechnique, INRIA), Thibaut Verron, Mohab Safey El Din and Jean-Charles Faugère (POLSYS, INRIA UPMC).

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In Vitro Physical experiments

Two test tubes are filled with matters which have the same NMR characteristics as two biological matters.

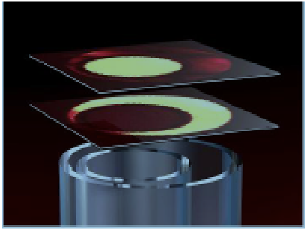

Figure: Simulation: interface oxygen./deoxygen. blood

(from Pr. Steffen Glaser Tech.Univ.München).

Physical experiments

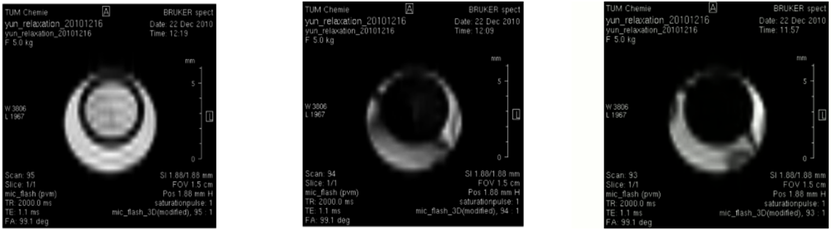

Figure: Simulation: interface oxygen./deoxygen. blood

Inner circle sample: mimics the deoxygenated blood.
Outside moon sample: simulates the oxygenated blood.

Physical experiments

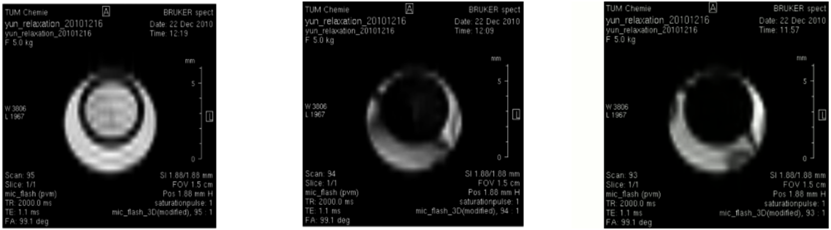

Figure: Simulation: interface oxygen./deoxygen. blood

Goal of the control: saturate the inner sample and maximize the remaining magnetization of the outside sample.

Physical experiments

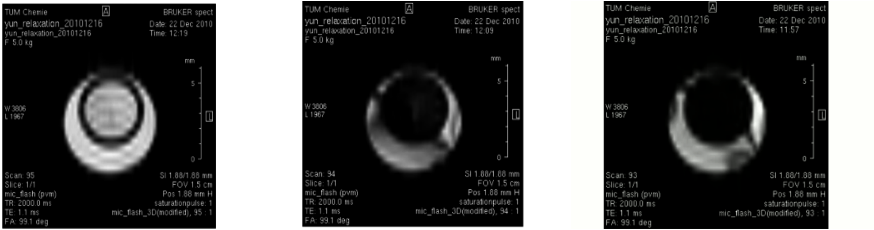

Figure: Simulation: interface oxygen./deoxygen. blood

Left: reference image after a short 90 degree pulse on both samples.

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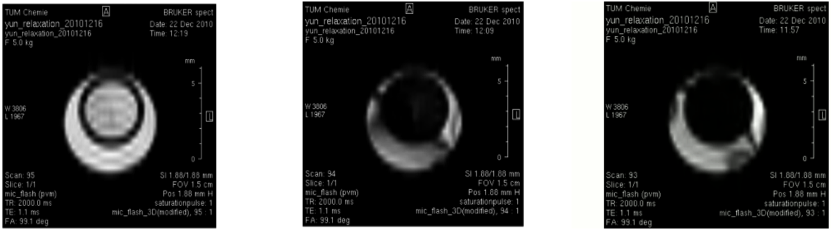

Figure: Simulation: interface oxygen./deoxygen. blood

Middle: remaining Y magnetization after the optimized pulse.

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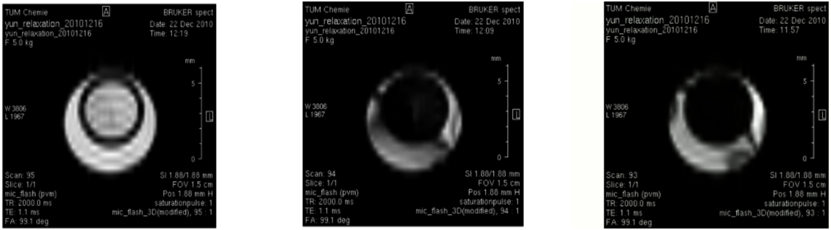

Figure: Simulation: interface oxygen./deoxygen. blood

Right: remaining Z magnetization after the optimized pulse.

Part II

A modelization : the Bloch model

Part II

The Bloch equation

Interface model

Mathematical contrast problem

Towards algebra : optimality conditions

The Bloch equation

Consider the vector field in $\mathbb{R}^3$

$$\begin{cases} \frac{dx}{dt} = -\Gamma x + u_y z \\ \frac{dy}{dt} = -\Gamma y - u_x z \\ \frac{dz}{dt} = \gamma(1 - z) + u_x y - u_y x \end{cases}$$

where

- $u = (u_x, u_y)$ is the control (magnetic field)
- $q = (x, y, z)$ is the magnetization vector
- (Γ, γ) are parameters.

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- (Γ, γ) are parameters.

Physical meaning of the parameters

- (Γ, γ) are related to the physical relaxation times T_1 and T_2
- $\gamma = \frac{1}{32.3 \cdot T_1}$
- $\Gamma = \frac{1}{32.3 \cdot T_2}$
- 32.3 Hz is the frequency of the magnetic field used in the NMR experiment

For instance (case 1):

- for water: $T_1 = T_2 = 2.5s$,
- for cerebrospinal fluid: $T_1 = 2s$, $T_2 = 0.3s$.

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Part II

Complete model with two Bloch equations

Since we are interested in the contrast provided by an interface (water/cerebrospinal fluid for instance), we consider a Bloch Eq. for each matter.

After normalization, we have a model in $\mathbb{R}^6$, formed by coupling two spin 1/2 particles, corresponding to two vector fields of the Bloch type

$$\begin{cases} B_1\dot{q}_1 = f(q_1) \\ B_2\dot{q}_2 = f(q_2) \end{cases}$$

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Reductions to 4D and single input

The control $u = (u_x, u_y)$ represents the magnetic field

In our normalization, its magnitude is bounded by $M = 2\pi$.

If we fix the control orientation, one can restrict each Bloch system to the 2D single-input case,

$$\begin{cases} \frac{dy_i}{dt} & = -\Gamma_i \, y_i - u_{x_i} \, z_i \\ \frac{dz_i}{dt} & = \gamma_i \, (1 - z_i) + u_{x_i} \, y_i . \end{cases} \qquad i = 1, 2$$

In short:

$$\dot{q} = F(q) + u \, G(q), \quad |u| \leq 2\,\pi$$

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Invariance of the Bloch ball under the dynamics

With our settings, the Bloch ball

$$\mathcal{B} = \{|q_1| \leq 1\} \times \{|q_2| \leq 1\}$$

is invariant for the dynamics, and the North pole $N = ((0,1),(0,1))$ is an equilibrium.

In all what follows we put the origin at the North Pole, and the center of the Bloch ball has new coordinates $(0,-1,0,-1)$.

Part II

Contrast problem by saturation

One considers two spin systems with state $q = (q_1, q_2)$, with relaxation parameters $(\Gamma_1, \gamma_1) \neq (\Gamma_2, \gamma_2)$, controlled by the same magnetic field. We play with the duration of the pulse, and the magnetic orientation at each time.

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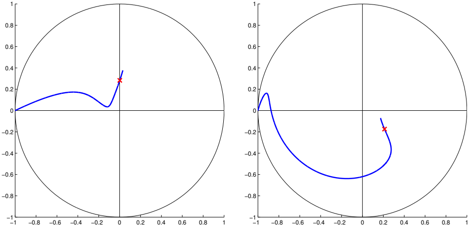

Figure: q_1 right, q_2 left (case 1).

Part II

Necessary optimality conditions

Proposition

$H(q,p,u) = \langle p, F(q) + uG(q) \rangle$ Hamiltonian lift of the system.

An optimal trajectory for the contrast problem must satisfy

- $\dot{q} = \frac{\partial H}{\partial p}, \quad \dot{p} = -\frac{\partial H}{\partial q}$
- $H(q,p,u) = \max_{|v| \leq M} H(q,p,v)$ *(maximization condition)*
- $q(0) = N, \quad q_1(T) = 0$ *(boundary conditions)*

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First approach : floating point computations

The first way of searching optimal trajectories is to use floating point packages

- there exist specialized and efficient packages devoted to Control Theory problems
- there are difficulties here because optimal policies are a sequence of Bang arcs and Singular arcs
- the number of B and S is not theoretically bounded (although in practice, the worst case seems to be BSBSBS)
- alternative approach : LMI techniques.
- difficult to have a global understanding of the problem.

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Singular case $H_G \equiv 0$

To understand the structure of the model we focus on the study of one special interesting case.
The singular case corresponds to $H_G \equiv 0$. We have (by the generalized Legendre–Clebsch condition):

$$\frac{\partial}{\partial u}\frac{d^2}{dt^2}\frac{\partial H}{\partial u} = \{H_G, \{H_G, H_F\}\} \le 0.$$

Furthermore $\tilde{M}(q,p) = \max_{|v|\le M} H(q,p,v)$ is constant on $[0, T]$ and if T is not fixed, one has $\tilde{M} \equiv 0$.

The case $\tilde{M} \equiv 0$ is called the exceptional case.

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Towards the algebraic problem

Introducing the determinants

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

Exceptional singular extremals (q, p) such that $\{\{H_G, H_F\}, H_G\} \neq 0$ project onto trajectories $q(\cdot)$ of the vector field $X_e = F - u_s^e G$ where $u_s^e = \frac{D'}{D}$ represents the singular feedback control.

On $\{D = 0\}$ the control explodes, but we can bypass this problem by desingularizing at points of $\{D = D' = 0\}$.

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Part III

Effective classification of four classical cases

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The four experimental cases

From the experimental point of view we are interested in four cases, with relaxation times T_1 and T_2 as follows:

1. water: $T_1 = T_2 = 2.5$; cerebrospinal fluid: $T_1 = 2$, $T_2 = 0.3$.
2. deoxygenated blood: $T_1 = 1.35$, $T_2 = 0.05$; oxygenated blood: $T_1 = 1.35$, $T_2 = 0.2$.
3. gray cerebral matter: $T_1 = 0.92$, $T_2 = 0.1$; white cerebral matter: $T_1 = 0.780$, $T_2 = 0.09$.
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To each of these cases correspond algebraic varieties $\{D = 0\}$ and $\{D' = 0\}$ associated to the control problem.

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Analytic expression of D

D equals

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

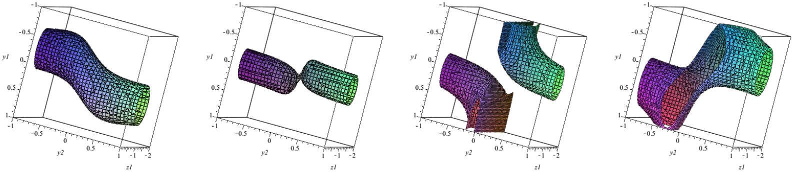

Figure: $\{D = 0\} \cap \{z_2 = \alpha\}$, $\alpha \in \{-0.5, -1, -1.16, -1.5\}$ (case 1).

Analytic expression of D'

D' equals

$$\begin{vmatrix} -\Gamma_1 y_1 & -(z_1+1) & -\Gamma_1 + (\gamma_1 - \Gamma_1) z_1 & -\Gamma_1^2 - (\gamma_1 - \Gamma_1)^2 z_1 \\ -\gamma_1 z_1 & y_1 & (\gamma_1 - \Gamma_1) y_1 & (\gamma_1 - \Gamma_1)^2 y_1 \\ -\Gamma_2 y_2 & -(z_2+1) & -\Gamma_2 + (\gamma_2 - \Gamma_2) z_2 & -\Gamma_2^2 - (\gamma_2 - \Gamma_2)^2 z_2 \\ -\gamma_2 z_2 & y_2 & (\gamma_2 - \Gamma_2) y_2 & (\gamma_2 - \Gamma_2)^2 y_2 \end{vmatrix}$$

is a degree 4 polynomial in (y_1, z_1, y_2, z_2).

Hypersurfaces $\{D = 0\}$ and $\{D' = 0\}$

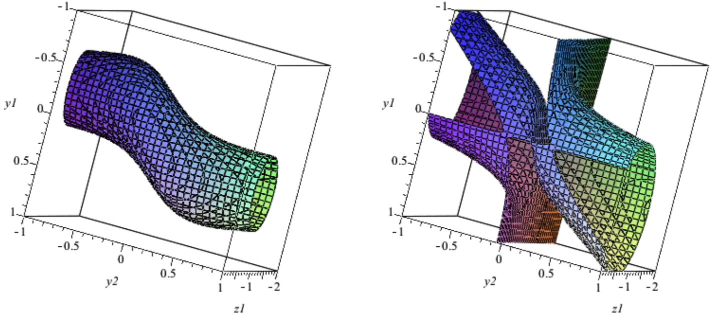

Figure: $z_2 = -0.5$, $\{D = 0\}$ left, $\{D' = 0\}$ right, case 1.

Hypersurfaces $\{D = 0\}$ and $\{D' = 0\}$

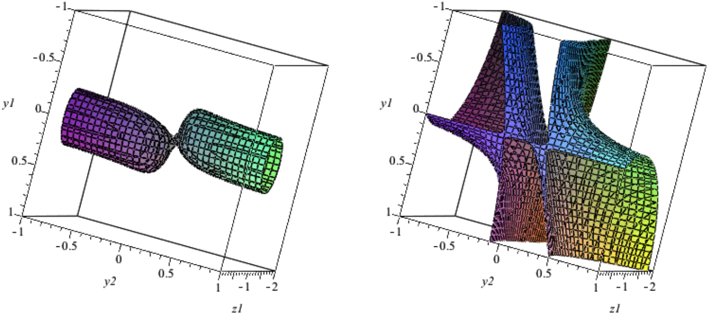

Figure: $z_2 = -1$, $\{D = 0\}$ left, $\{D' = 0\}$ right, case 1.

Hypersurfaces $\{D = 0\}$ and $\{D' = 0\}$

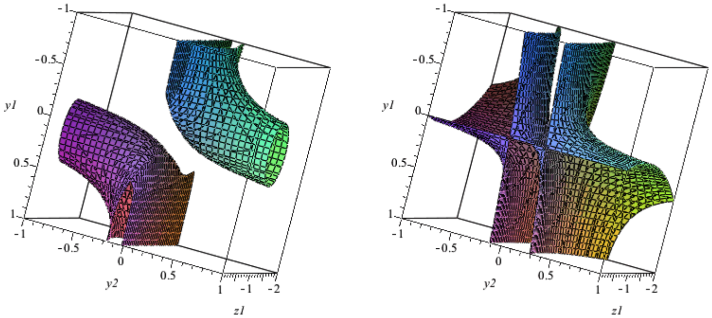

Figure: $z_2 = -1.16$, $\{D = 0\}$ left, $\{D' = 0\}$ right, case 1.

Hypersurfaces $\{D = 0\}$ and $\{D' = 0\}$

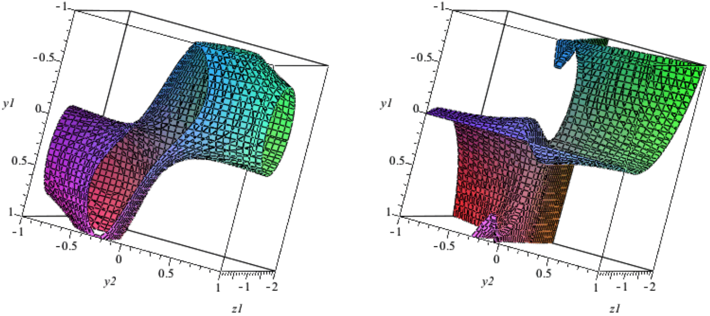

Figure: $z_2 = -1.5$, $\{D = 0\}$ left, $\{D' = 0\}$ right, case 1.

Classification criteria

As far as we know, there are no theoretical invariants for the intersection of two quartics in 4D inside an algebraic 4D ball.

We build our own classification that will depend on the study of:

- the singularities of $\{D = 0\}$
- the intersection surface $\{D = 0\} \cap \{D' = 0\}$
- the curve Σ of the singularities of $\{D = 0\} \cap \{D' = 0\}$

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This is done first by means of algebraic computations involving Gröbner bases, and further semi-algebraic computations to take into account the Bloch ball.

Part III

Singularities of $\{D = 0\}$

We have to solve the algebraic system $\{D = 0, \nabla D = 0\}$.

- with floating points coefficients, the numerical instability is so high that one gets inconsistent results
- to solve the system, we compute with rational coefficients, that is, with infinite precision, and we reduce the system by means of computing a Gröbner basis.
- this is sufficient to separate the four experimental cases, but provides very few information.

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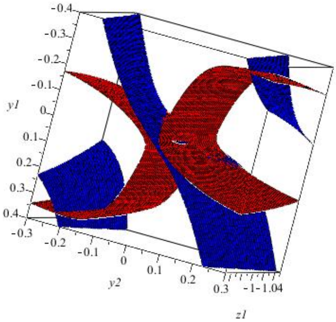
Singularity of $\{D = 0\}$ at the center of the Bloch ball



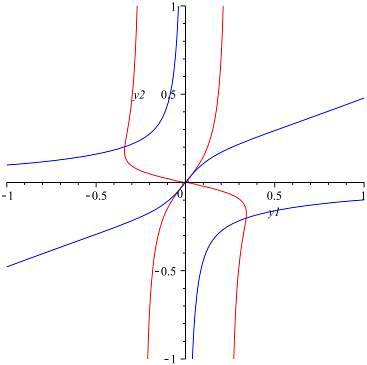


Figure: Singularity at the center of the Bloch ball O, case 1.

Part III

Classification of the experimental cases

Singularities of $\{D = 0\}$

Intersections

Singular intersection

The surface $\{D = 0\} \cap \{D' = 0\}$

This surface is of particular interest because of the expression of the desingularized vector field.

We have to solve the algebraic system $\{D = 0, D' = 0\}$.

Here also we reduce the system by means of computing Gröbner bases

The intersections are defined by means of explicit rational/implicit formulas.

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We have to solve the algebraic system

$$\{D = 0, D' = 0, M_2(\nabla D, \nabla D') = 0\}$$

where M_2 are the 2×2 minors of the matrix $[\nabla D, \nabla D']$.

Factorized Gröbner bases are involved in these computations, rotating the orderings to get different projections of the algebraic curve Σ.

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Comparison of the cases by means of Σ

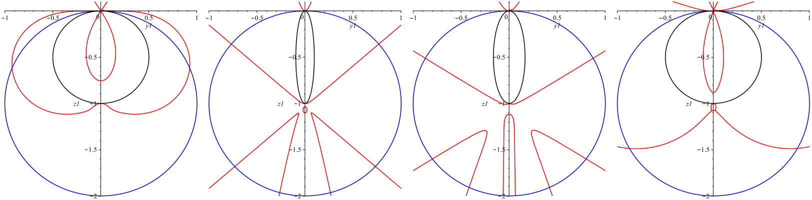

Figure: Projection on (y_1, z_1) of the singular line Σ, intersections with the Bloch sphere, cases 1-4.

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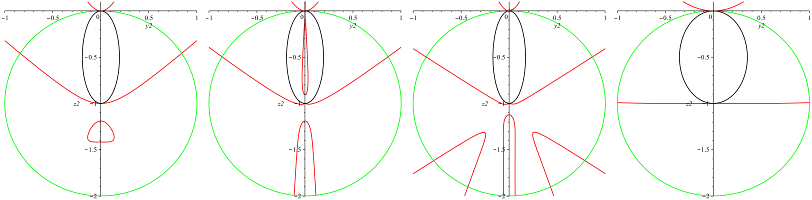

Figure: Projection on (y_2, z_2) of the singular line Σ, intersections with the Bloch sphere, cases 1-4.

At this point, we are able to compute all the information for any given set of parameters.

Part IV

The general classification problem

Part IV

Bifurcations of the singularities of $\{D = 0\}$

Case of water and another matter

Bifurcations with respect to the parameters

The next step of our analysis is to consider the above problems (for instance singularities) when $(\gamma_1, \Gamma_1, \gamma_2, \Gamma_2)$ are free variables.

For instance if one considers the singularity system $S =< D = 0, \nabla D = 0 >$, how does the number of real roots bifurcate inside the Bloch ball, and how does the number of complex roots bifurcate ?

Many bifurcations are expected, since we can observe strong degeneracies when the parameters vanish, when $\gamma_i = 2\Gamma_i$, as well as when $\gamma_1 = \gamma_2$ (which includes the blood case).
Are there other bifurcations ?

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Bifurcations of the algebraic singularity problem

The problem is reducible by homogeneity in the parameters space, fixing $\gamma_1 = 1$.

We have a degree 4 system in $q = (y_1, z_1, y_2, z_2)$ with 3 free parameters.

The easy case is to find the singularities on $\{y_1 = y_2 = 0\}$. The difficult case is to find the singularities outside this plane.

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Singularities on $\{y_1 = y_2 = 0\}$

On $\{y_1 = y_2 = 0\}$ the computing of a Gröbner basis is of course much easier. One gets the singularity $(0, -1, 0, -1)$ and (provided denominators $\neq 0$) another explicit singularity $(0, z_1, 0, z_2)$ with

$$z_1 = \frac{(2\,\Gamma_1 - 1)\,(\Gamma_2 - \Gamma_1)}{(3 - 2\,\Gamma_1)\,\Gamma_2 + 2\,\Gamma_1^2 - 3\,\Gamma_1 - \gamma_2 + 1}$$

$$z_2 = \frac{(2\,\Gamma_2 - \gamma_2)\,(\Gamma_2 - \Gamma_1)}{\gamma_2 - \gamma_2^2 - 2\,\Gamma_2^2 + (2\,\Gamma_1 + 3\,\gamma_2)\,\Gamma_2 - 3\,\Gamma_1\,\gamma_2}$$

It is easy to determine the position of this singularity in the Bloch ball.

Singularities outside $\{y_1 = y_2 = 0\}$

After blowing-up $y_1 = t\, y_2$, appears a natural reduction $Y_2 = y_2^2$.

To compute a Gröbner basis for the new system $\hat{S}$, one has to compute in two steps, with blocks-orderings on

$$[c, y_2][z_1, z_2, t, Y2, \Gamma_1, \Gamma_2, \gamma_2],$$

and then on

$$[c, y_2, z_1, z_2, t][Y2, \Gamma_1, \Gamma_2, \gamma_2]$$

(c is a saturation variable).

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Singularities outside $\{y_1 = y_2 = 0\}$

A Gröbner basis for $\hat{S}$ has the following properties

- It contains a polynomial $p_4 \in \mathbb{Z}[\Gamma_1, \gamma_2, \Gamma_2][Y_2]$ of degree 4 in Y_2,
- p_4 has 1776 monomials,
- p_4 may have 0 to 4 real roots, and for generic $(\Gamma_1, \gamma_2, \Gamma_2)$ there are 4 complex roots,
- the reality of the roots of p_4 is discussed readily from the positivity of the root $Y2$,
- p_4 has a linear factor when $\Gamma_1 = 1$ or $\Gamma_2 = \gamma_2$ (corresponds to water),
- the discussion on the roots of the system induces 10 different cases.

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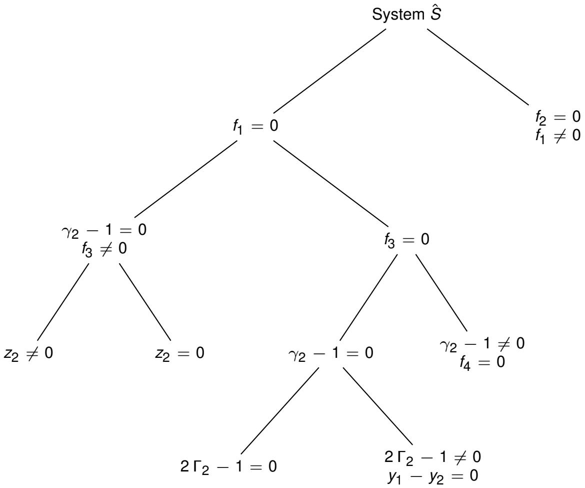
Complete Resolution Tree for system $\hat{S}$



Part IV

Bifurcations of the singularities of $\{D = 0\}$

Case of water and another matter

The case of water and another matter

The question is to detect metabolites in rat brains. The experiments will soon be achieved *in vivo* with 4T or even 11T.

In the case of water, $\gamma_1 = \Gamma_1$, and by homogeneity $\gamma_1 = \Gamma_1 = 1$.

For singularities on the plane $y_1 = y_2 = 0$ we get very simple explicit formulas

$$z_1 = \frac{\Gamma_2 - 1}{\Gamma_2 - \gamma_2}$$

$$z_2 = \frac{(2\,\Gamma_2 - \gamma_2)\,(1 - \Gamma_2)}{(2\,\Gamma_2 - \gamma_2 - 2)\,(\Gamma_2 - \gamma_2)}$$

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The case of water

Outside this plane, we get (with $\gamma_2 = h\,\Gamma_2$) a two-parameters solution

$$z_1 = \frac{(\Gamma_2\,h + \Gamma_2 - 1)\,(1 - \Gamma_2)}{(4\,\Gamma_2\,h - 5\,\Gamma_2 - 1)\,\Gamma_2\,(h - 1)}$$

$$z_2 = \frac{1}{2}\frac{(1 - \Gamma_2)\,(h - 2)}{(\Gamma_2\,h + \Gamma_2 - 1)\,(h - 1)}$$

$$y_2 = \pm\frac{1}{2}\,\frac{h\sqrt{3}\sqrt{\Gamma_2\,(\Gamma_2 - 1)\,(h - 2)\,(2\,\Gamma_2\,h - \Gamma_2 - 1)\,(2\,\Gamma_2\,h - \Gamma_2 - 2)}}{(\Gamma_2\,h + \Gamma_2 - 1)\,(h - 1)\,(2\,\Gamma_2\,h - \Gamma_2 - 2)}$$

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(with abusive square roots).

The case of water

There are two other one-parameter families of solutions, corresponding to complex singularities:

- the first family

$$\gamma_2 = 2 - \Gamma_2 \quad z_1 = \frac{1}{4}\,\frac{\Gamma_2}{1-\Gamma_2} \quad z_2 = \frac{1}{4}\,\frac{3\,\Gamma_2 - 2}{1-\Gamma_2}$$

$$t = \frac{3\,\Gamma_2 - 2}{2-\Gamma_2} \quad Y_2 = -\frac{1}{16}\,\frac{(\Gamma_2-2)^2}{(\Gamma_2-1)^2}$$

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- the second family

$$\Gamma_2 = -\frac{1}{6}\,\frac{\sqrt{2}\left(5\,u^2+6\,u+5\right)}{u^2-1} \qquad \gamma_2 = -\frac{2}{3}\,\frac{\sqrt{2}\left(u^2+1\right)}{u^2-1}$$

$$Y_2 = -8\,\frac{\left(3+2\sqrt{2}\right)(u+1)^2\left(u^2+1\right)^2}{\left(-u-3+2\sqrt{2}\right)^2\left(u+3+2\sqrt{2}\right)^4}$$

$$t = \frac{3}{4}\,\frac{(u-1)^2}{u^2+1}$$

$$z_1 = -\frac{1}{46}\,\frac{\left(3\sqrt{2}+8\right)\left(14\sqrt{2}u^2-23\,u^3-36\sqrt{2}u-45\,u^2-10\sqrt{2}-65\,u-27\right)}{\left(-u-3+2\sqrt{2}\right)\left(u+3+2\sqrt{2}\right)^2},$$

$$z_2 = -\frac{1}{7}\,\frac{\left(2\sqrt{2}+1\right)\left(-u+3+2\sqrt{2}\right)\left(-7\,u-9+4\sqrt{2}\right)(u+1)}{\left(-u-3+2\sqrt{2}\right)\left(u+3+2\sqrt{2}\right)^2}$$

Bifurcation diagram of the singularities

The fact that we get explicit formulas is very important, in order to

- find the bifurcations
- (later) find normal formal forms for the vector fields near these singularities.

Bifurcations occur when one solution crosses the circle $y_1^2 + (z_1 + 1)^2 = 1$, resp. $y_2^2 + (z_2 + 1)^2 = 1$, and when the square roots or the denominators vanish: this is an algebraic set Θ in (γ_2, Γ_2)

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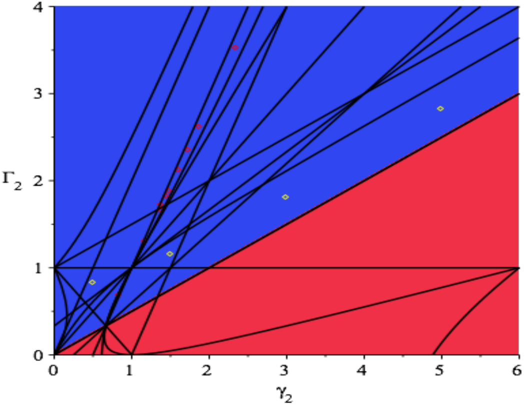
Bifurcation diagram of the singularities

We proceed to a Cylindric Algebraic Decomposition of the complementary of Θ and just get 14 test points corresponding to real singularities in the Bloch ball.



Classification by means of Σ

By means of explicit formulas and CAD, all the configurations are known. Among them:

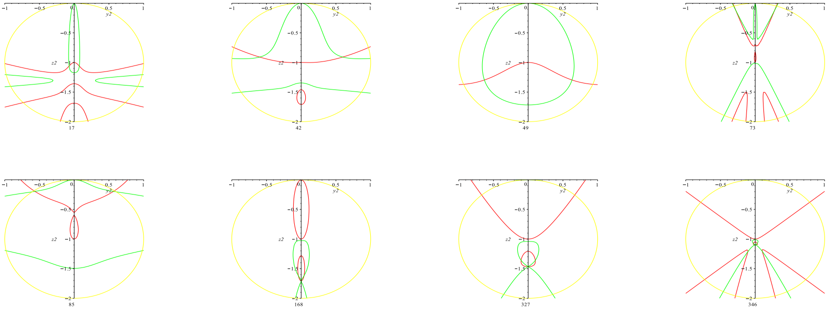


Figure: Projection on (y_2, z_2) of the singular line Σ, intersections with the Bloch sphere, some cases with water.

Conclusion

We expect to understand everything of the structure of the algebraic problem, not only singularities, but also the intersection $\{D = 0\} \cap \{D' = 0\}$ and the curve Σ.

This goal is already achieved in the case of water, and just remains the computation of Σ in the general case.

Our long term aim is to use this information to better understand the dynamics, build normal forms of the vector field and improve numerical algorithms.

This kind of methods can be used in other Control Theory problems (for instance Protein Misfolding Cyclic Amplification - prion diseases).

Conclusion

We expect to understand everything of the structure of the algebraic problem, not only singularities, but also the intersection $\{D = 0\} \cap \{D' = 0\}$ and the curve Σ.

This goal is already achieved in the case of water, and just remains the computation of Σ in the general case.

Our long term aim is to use this information to better understand the dynamics, build normal forms of the vector field and improve numerical algorithms.

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