Working example 1 Geometric optimal control and the contrast problem in NMR and MRI

June 17, 2015

Model (Bloch equations in NMR)

$$\frac{dM}{d\tau} = \gamma M \wedge B + R(M)$$

- γ : gyromagnetic ratio
- $B = (B_x, B_y, B_z)$ magnetic field : (B_x, B_y) Rf-control field, $B_z = B_0 + \Delta B_0$ with B_0 strong polarizing field and ΔB_0 is used in MRI to localize a pixel
- $R(M) = -(M_x/T_2, M_y/T_2, (M_z - M_0)/T_1)$, M magnetization vector of the spin, T_1, T_2 relaxation parameters which are the signature of the chemical species (water, fat, bloodetc....) : dissipation term of Lindblad equations.

First normalization

Rescale $(M_x, M_y, M_z) \to (M_x/M_0, M_y/M_0, M_z/M_0)$ to identify $M_0 = 1$

Set $\omega_0 = -\gamma B_0$ (resonance frequency), $u(\tau) = -\gamma B_y, v(\tau) = -\gamma B_x$ (control components) so that Bloch equation is written in the form

$$\frac{dM_x}{d\tau} = -\omega_0 M_y + u M_z - M_x/T_2$$

$$\frac{dM_y}{d\tau} = -v M_z + \omega_0 M_x - M_y/T_2$$

$$\frac{dM_z}{d\tau} = -u M_x + v M_y - (M_z - 1)/T_1$$

Resonance for the mathematician

Introduce the rotating frame

$$\Omega_z = \begin{pmatrix} 0 & -1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

$$S(\tau) = exp\omega\tau\Omega_z$$

and perform the change of coordinates

$$M = S(\tau)q, q = (x, y, z).$$

Hence the Bloch equations take the form

$$\frac{dx}{d\tau} = -\Delta\omega y + u_2 z - x/T_2$$

$$\frac{dy}{d\tau} = \Delta\omega x - u_1 z - y/T_2$$

$$\frac{dz}{d\tau} = -u_2 x + u_1 y - (z-1)/T_1$$

where $\Delta\omega = \omega_0 - \omega$ is the resonance offset
and gthe Rf field is in the resonant representation

$$u_2 = ucos\omega\tau - vsin\omega\tau, u_1 = usin\omega\tau + vcos\omega\tau$$

Interpretation

At resonance $\omega = \omega_0$ the strong magnetization field B_0 is no more visible and only the Rf field acts in the resonant representation

Normalization

Use a normalize time t such that the control bounds is 2π to get our working equations

$$\frac{dx}{dt} = -\Gamma x + u_2 z$$

$$\frac{dy}{dt} = -\Gamma y - u_1 z$$

$$\frac{dz}{dt} = \gamma(1-z) + u_1 y - u_2 x$$

With

- q belongs to the unit ball called the Bloch ball provided : $2\Gamma \geq \gamma > 0$
- The physical parameters are renomalized in the time reparameterization.

Color convention in MRI

Attribute to $\mid q \mid$ a level of grey such that $\mid q \mid= 1$ corresponds to white and $\mid q \mid= 0$ to black (which correspond to no signal) .

Saturation problem in NMR

It is a fundamental problem of driving the system from the north pole of the Bloch ball tp the center O so that the NMR signal is zero. The important question is to make this saturation inb minimum time.

A standard control sequence to make this satuation is to invert ths spin to the south pole and let the system relax along the z-axis. An important contribution od f optimal control was to compute the time minimal sequence that we explain next.

First of all due to th sysmetry of revolution of the system we can restrict to the single input case

$$\frac{dy}{dt} = -\Gamma y - u_1 z$$

$$\frac{dz}{dt} = \gamma(1 - z) + u_1 y.$$

The main point from geometric control theory is to compute the singular trajectories. The system is written

$$\frac{dq}{dt} = F_0(q) + u_1 F_1(q).$$

In dimension 2 using the contraints $\{H_1 = \{H_1, H_0\} = 0$ one gets that they are contains in the set

$$\Sigma' : det(F_1, [F_1, F_0]) = 0$$

which forms the two lines

- $y = 0$ (axis of revolution)
- $z_0 = -\frac{\gamma}{2(\Gamma-\gamma)} == -\frac{T_2}{2(T_1-T_2)}$.

The interesting situation is when $2\Gamma > 3\gamma$ so that the horizontal line intersects the Bloch ball. The limit time minimal synthesis using control impulses rather than bang arcs is to follows this line up to the z-axis and let the system relax along the vertical line using a zero control. The total amount time needed along the singular horizontal and the vertical lins represents the physical limit to saturate and depends of the position of z_0 which is the main invariant of the problem. Since the control is bounded by 2π there are conditions such that the singular control is admissible. Also along the singular horizontal line the control is blowing up when $y_s \to 0$ so that this line has to be quitted a single point prior the control saturation. This phenomenon is called a bridge phenomenon and the corresponding bang solution is called a bridge.

We have

Proposition

Provide $2\Gamma > 3\gamma$ and the singular horinzontal line is admissible the time minimal solution is of the form $\sigma_+\sigma_s\sigma_+^B\sigma_s$ where σ_s are singular arcs and σ_+ are bang arcs with $u_1 = 2\pi$ and the indice B represents the bridge.

Note

This discussion which is rather simple in the context of geometric optimal control has to be generalize in the double saturation problem and in the contrast problem in NMR.

Double saturation problem

Take a pair of such 2D-systems coupling two spins with differents relaxations parameters $(\gamma_1, \Gamma_1), (\gamma_2, \Gamma_2)$ find the time minimal policy to drive the two spins from the north pole to the center of the respective Bloch balls.

Contrast by saturation in NMR

Take a pair of such 2D-systems coupling two spins with differents relaxations parameters $(\gamma_1, \Gamma_1), (\gamma_2, \Gamma_2)$ find the optimal policy for in a given time steers the first spin to zero (saturation) while maximizing the amplitude of the second spin to provide a maximum contrast in the imagd corresponding to this amplitude.

Contrast problem by saturation in MRI taking into account the B_0 and B_1 (Rf) inhomogeneities

The principle of MRI is to work with a sequence of spins localized in space (position of the pixel on the image) where focus on a specific pixel at position x is obtained by modified the field B_0 as $B_0 + x\Delta B_0$ to modified the resonant frequency associated to such a field and select the appropriate pixel. Unfortunalty this property which allows to produce the image ha a bad consequence since they are variations of the B_0 and the B_1 due to the process and moreover they can be only measured and not modeled. Hence due to those homogeneities the computed Rf-field has not exact computed effect on the image contrast and as a second step a so-called robust sequence has to be computed to compensate the effect of inhomogeneities. This can be easily modeled using the Bloch equations. For the analysis it is better to separate the B_0 and B_1 inhomogeneities.

B_0 inhomogeneities

According to our model the role is clear because it amounts only to introduce a detuning term $\Delta\omega$ in our equation centered with respect to the perfect value ω_0. Clearly it has a strong effect to the ideal contrast policy in NMR and in particular we cannot restrict our study to the single input case. Fortunatly the objects of geometric optimal control are suitable to handle this modification of the system.

B_1 inhomogeneities

Again using our model such inhomogeneity amount only to a variation of the amplitude of the applied Rf field depending upon the localization of the spin in the image.

Note

In both cases they are to be experimentally computed that is there is no special relation between such inhomogeneities and the position of the spin in the image.

Geometric tools in the classification of singular trajectories in relation of the action of the feedback group

Two distinct motivations

Motivation 1

Analyze the singular flow in relation of the computation of the optimal strategy in the contrast problem : number of bang arcs mainly related to the blowing up of ther singular control due to the singular set $< p, [[F_1, F_0], F_1] >= 0$.

Motivation 2

Relate the physical parameters to the invariant for the feedback group

Program 1 Classification of the singular flow in relation with motivation 1

Notations

$$\frac{dq}{dt} = F_0 + uF_1, q\epsilon M \to (F_0, F_1)$$

Feedback goup (local or global)
* Change of coordinates : $q = \varphi(Q)$ action on vector fields (tensors)

- $$\varphi * F = \frac{\partial \varphi^{-1}}{\partial Q} F o \varphi(Q)$$

  image vector field. Acts on systems as

$$(F_0, F_1) \to (\varphi * F_0, \varphi * F_1)$$

*Feedback $u = \alpha(q) + \beta(q)v, \beta \neq 0$

$$(F_0, F_1) \to (F_0 + u\alpha, F_1\beta)$$

Note $F_1 \to F_1\beta$: classification of the distribution

* Singular flow : $z = (q, p)$ Darboux coordinates on the cotangent bundle , that is

$$\omega = dq \wedge dp$$

* Symplectic lift of the vector field F : $< H(z) =< p, F(q) >$ of the system

$$\frac{dz}{dt} = \mathbf{H}_0 + u\mathbf{H}_1$$

* Symplectic lift of a diffeomorphism φ (Mathieu transformation) :

$$q = \varphi(Q), p = P\frac{\partial \varphi^{-1}}{\partial Q}$$

NB line notation for the adjoint vectors

* Singular trajectories system : lift the system into

$$\frac{dz}{dt} = \mathbf{H_0}(z) + \mathbf{H_1}(z)$$

Constraints

$$\Sigma : H_1 = 0$$

$$\Sigma' : H_1 = \{H_1, H_2\} = 0$$

Singular control given by

$$\{\{H_1, H_0\}, H_0\} + u_s\{\{H_1, H_0\}, H_1\} = 0$$

If $\{\{H_1, H_0\}, H_1\} \neq 0$ define the Hamilonian

$$H_s =< p, F_0(q) + u_s(z)F_1(q) >$$

Note : Only the solutions in Σ' have an invariant meaning

Notations

- Lie bracket $[F,G\}(q)=\frac{\partial F}{\partial q}(q)G(q)-\frac{\partial G(q)}{\partial q}F(q)$
- Poisson bracket $\{H,G\}=dH(\mathbf{G})$
- H_i hamiltonian lifts : $\{H_0,H_1\}(z)=<p,[F_0,F_1]>$.

The surface Σ'

$$<p,F_1(q)>=<p,[F_0,F_1](q)>=0$$

Notation

K the set where : $\{q,F_1,[F_0,F_1]\}$ are independent

Properties

- K is feedback invariant and hence an invariant meaning
- Since $p\neq 0$ the surface Σ' is of codimension 2 outside K.

Analysis outside K

Computations

$$F_1\neq 0, F_1=\frac{\partial}{\partial q_1}, F_0=F_0^1\frac{\partial}{\partial q_1}+F_0'\frac{\partial}{\partial q'}$$

$$q=(q_1,q'), p=(p_1,p')$$

$$<p,F_1>=0\Rightarrow p_1=0$$

$$[F_0,F_1]=\frac{\partial F_0}{\partial q_1},[[F_0,F_1],F_1]=\frac{\partial^2 F_0}{\partial q_1^2}.$$

$$S:(q,p)\epsilon\Sigma',<p,[[F_0,F_1],F_1]>=0$$

Surface Σ' .
Outside S solve $<p',\frac{\partial F_0'}{\partial q_1}>=0$ using the implicit function theorem

$$q_1=f(q',p'), p_1=0.$$

Note : the surface Σ' is of codimension 2 if $F_1\neq 0$ and $\{H_1,H_0\},H_1\}$

Notation

Note H'_s the restriction of H_s the surface $\Sigma' \setminus S$ outside K

Claim

The Hamiltonian vector field $\mathbf{H}'_s$ for the restriction of ω to this surface describes the explicit representation of the singular trajectories by an hamiltonian vector field

Computations

-
$$< p, F >= p.F = P\frac{\partial \varphi^{-1}}{\partial Q}F(\varphi(Q)) = P.\varphi * F = H_{\varphi * F}$$

$$[\alpha(q)F, G] = \alpha[F, G] + (L_G\alpha)F$$

Applications

- Σ : feedback invariant
- Σ' : feedback invariant
- S : feedback invariant

Note

Change of coordinates φ acts on functions defining the surfaces as composition by the symplectic lift (Mathieu transformation)

Stratification

-
$$D_1 = spanF_1$$
-
$$D_2 = span\{F_1, [F_0, F_1]\}$$
-
$$D_3 = span\{F_1, [F_0, F_1], [[F_0, F_1], F_1]\}$$

- $\Sigma : F_1 = 0$
- $F_1 \neq 0$,
- Σ' : $[F_0, F_1] = 0$,
- $[F_0, F_1] \neq 0$, $\{F_1, [F_0, F_1]\}$ collinear $\rightarrow$ set K
- Σ'': $F_1, [F_0, F_1]$ independent and dim $D_3 < 3$ (SVD test ?)

Note

F_1 can be linearized to $\frac{\partial}{\partial q_1}$ using polar coordinates (alternative coordinates Lie bracket computations)

Singular flow desingularization

$$\frac{dz}{dt} = \{\{H_0, H_1\}, H_1\}\mathbf{H}_0 - \{\{H_0, H_1\}, H_0\}\mathbf{H}_1$$

Fact

Semi covariant using the singular flow for the feedback classification reduced to the action of Mathieu transformations

Program 2 Relate the physical parameters to the feedback invariants

This is a different program (although not completly independent) where one must generate a complete set of invariants for the action of the feedback group in relations with the physical parameters. More precisely rational invariants will be deduced form the analysis of the singular flow. A first technique to handle this problem is to retsrict the feedback classification to the singular trajectories contained in the level set $H_0 = 0$.

Indeed using this additional constraint the singular trajectories defined a vector field on the state space only and the feedback cllassification reduced to classify this vector field using change of coordinates only.

From the computation of the optimal solution this amounts to analyze the contrast problem but with a non fixed transfer time.

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