Geometric Control and Homotopic Methods for solving a Bang-Singular problem

Applied and Numerical Optimal Control
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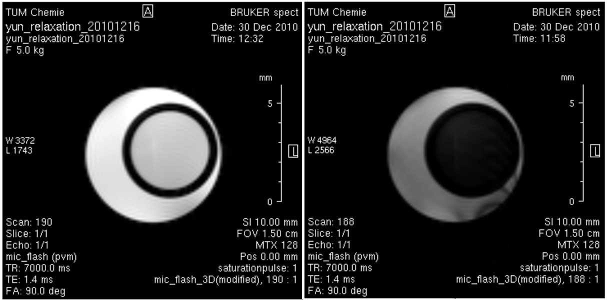

Figure: (LHS) Hard pulse of 90°. (RHS) Optimal solution.

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Contrast problem

$$(P)\left\{\begin{array}{l} |q_2(t_f)|^2 = \left(y_2^2(t_f) + z_2^2(t_f)\right) \to \max \\ \left[\begin{array}{lcl} \dot{y}_1 & = & -\Gamma_1 y_1 - u z_1 \\ \dot{z}_1 & = & \gamma_1(1-z_1) + u y_1 \end{array}\right. \\ \left[\begin{array}{lcl} \dot{y}_2 & = & -\Gamma_2 y_2 - u z_2 \\ \dot{z}_2 & = & \gamma_2(1-z_2) + u y_2 \end{array}\right. \\ q_1(0) = (0,1) = q_2(0) \\ q_1(t_f) = (0,0) \end{array}\right.$$

$$q_i = (y_i, z_i),\ |q_i| \leq 1,\ i = 1,2$$

$$\gamma_i = 1/(32.3 T_{i1}.10^{-3})$$
$$\Gamma_i = 1/(32.3 T_{i2}.10^{-3})$$

$$|u| \leq 2\pi$$

Spin 1 (y_1, z_1) -	Deoxygenated blood	: $T_{11} = 1350$ ms,	$T_{12} = 50$	ms
Spin 2 (y_2, z_2) -	Oxygenated blood	: $T_{21} = 1350$ ms,	$T_{22} = 200$	ms
Spin 1 (y_1, z_1) -	Cerebrospinal fluid	: $T_{11} = 2000$ ms,	$T_{12} = 200$	ms
Spin 2 (y_2, z_2) -	Water	: $T_{21} = 2500$ ms,	$T_{22} = 2500$	ms

Blood: $T_{min} = 6.7980978$
Fluid: $T_{min} = 20.2301921$

Pontryagin Maximum Principle

- We have a (smooth) Mayer problem of the form:

$$\min_{u \in \mathcal{U}} c(q(t_f)), \quad \dot{q} = F(q) + uG(q), \quad q = (q_1, q_2) \in \mathbb{R}^4, \quad |u| \leq 2\pi, \ u \in \mathbb{R},$$

  where
  - $c(q(t_f)) = -\left(y_2^2(t_f) + z_2^2(t_f)\right)$
  - $F(q) = \sum_{i=1,2} (-\Gamma_i y_i) \frac{\partial}{\partial y_i} + (\gamma_i(1 - z_i)) \frac{\partial}{\partial z_i}$
  - $G(q) = \sum_{i=1,2} -z_i \frac{\partial}{\partial y_i} + y_i \frac{\partial}{\partial z_i}$

- The Hamiltonian is: $H(q,p,u) = \langle p, F(q) + uG(q) \rangle$

- And the Maximum Principle gives: $\begin{cases} u = 2\pi \, sign(H_G) \text{ is bang} & \text{if } H_G \neq 0 \\ u \text{ is singular} & \text{if } H_G = 0 \end{cases}$

- The boundary conditions are:

$$q_1(t_f) = 0 \quad \text{(zero magnetization of the first spin)}$$

$$p_2(t_f) = -2p^0 q_2(t_f), \quad p^0 \leq 0.$$

Simplest possible solution

- The north pole $N = ((0,1),(0,1)) = x(0)$, is an equilibrium point for the singular control system ($u_s = 0$): start with a bang.
- Due to symmetry of revolution: the first bang is either $u = +2\pi$ or $u = -2\pi$.
- A bang solution amounts roughly to a rotation of each plane (y_i, z_i) around 0.
- At t_f, $q_1(t_f) = 0$, and there is no improvement by rotation (because $T_{21} > T_{22}$) of the contrast: no bang at the end.

Lemma

The simplest BC-extremal in the contrast problem is of the form B^+S.

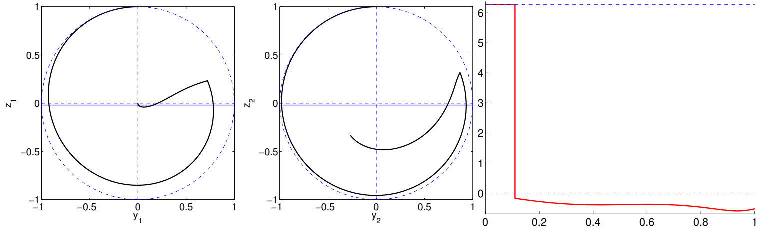


Figure: Trajectories of spin 1, 2 and the control associated for the Blood case.

The Hamiltonian is $H(q,p,u) = H_F(q,p) + u\,H_G(q,p)$, $H_F := \langle p, F\rangle$, $H_G := \langle p, G\rangle$.

Let $z(\cdot) = (q(\cdot), p(\cdot))$ be a singular extremal, then $H_G(z(.)) = 0$ identically.
Differentiating with respect to time,

$$\left.\begin{aligned} & H_G(z(t)) = 0 \\ \frac{dH_G}{dt}(z(t)) = \{H, H_F\}(z(t)) = & \{H_G, H_F\}(z(t)) = 0 \end{aligned}\right\} \text{(2 constraints)}$$

$$\frac{d^2H_G}{dt^2}(z(t)) = \{\{H_G, H_F\}, H_F\}(z(t)) + u_s(t)\{\{H_G, H_F\}, H_G\}(z(t)) = 0$$

Besides,

- we can restrict p to $H_s = h$ because of the homogeneity : $u_s(q, \alpha p) = u_s(q,p)$.
- generalized Legendre-Clebsch condition has to be satisfied that is $\{\{H_G, H_F\}, H_G\} \geq 0$.

$\Rightarrow$ for each $q(0) \in \mathbb{R}^4$, $p(0) \in \mathbb{R}^4$ lives in half a straight line and the singular flow starting from $q(0)$ is a surface of dimension 2.

Singular extremals in the Fluid case

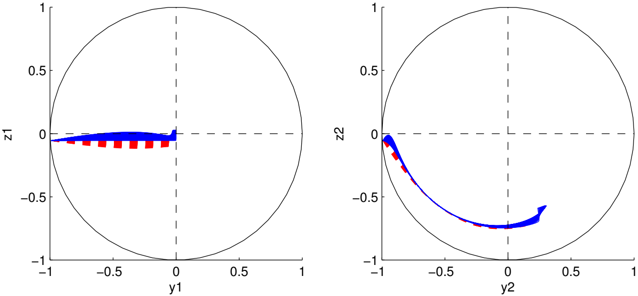


Figure: Singular surface with blowing up control in red ($\{\{H_G, H_F\}, H_G\}$ tends to 0).

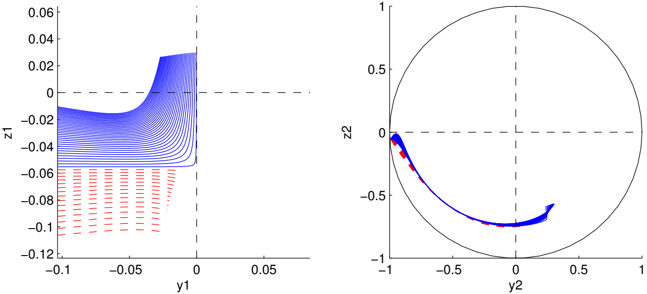


Figure: Zoom of singular surface with blowing up control in red ($\{\{H_G, H_F\}, H_G\}$ tends to 0).

Local optimality of singular arcs

Définition

Let $z(\cdot)$ be a reference singular solution of $\vec{H}_s$ on $[0, t_f]$. The variational equation on the tangent space to $\Sigma_s := \{H_G = \{H_F, H_G\} = 0\}$

$$\dot{\delta z} = d\vec{H}_s(z(t))\delta z$$
$$dH_G = d\{H_F, H_G\} = 0$$

is called Jacobi equation.

- *A Jacobi field $J(t) = (\delta q, \delta p)$ is a non-zero solution of Jacobi equation.*
- *It is said semi-vertical at time t if $\delta q(t) \in \mathbb{R}G(q(t))$.*
- *A time $t \in (0, t_f]$ is said to be conjugate if there exists a Jacobi field $J(t)$ semi-vertical at 0 and t.*

Theorem

Under strict Legendre-Clebsch condition (i.e. $\{\{H_G, H_F\}, H_G\} > 0$) and additional generic assumptions, the absence of conjugate times on $(0, t_f)$ is necessary for local optimality of a singular arc.

Conjugate points fot singular extremals in the Fluid case

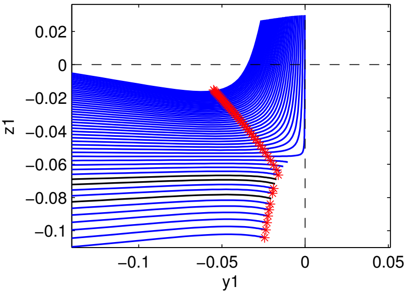


Figure: Zoom of singular surface with conjugate points in red.

$\Rightarrow$ We can expect more intricate structures than BS in the fluid case.

The limit case $t_f = T_{min}$. Single spin problem (see [BCG+11])

$$
(P_1) \begin{cases} t_f \to \min \\ \left[\begin{array}{lcll} \dot{y} & = & -\Gamma y & - u z \\ \dot{z} & = & \gamma(1-z) & + u y \end{array} \right. \\ q(0) = (0,1) \\ q(t_f) = (0,0) \end{cases}
$$

$$q = (y,z), \; |q| \leq 1$$

$$\frac{3\gamma}{2} < \Gamma$$

$$|u| \leq 2\pi$$

The dynamics: $\dot{q} = F(q) + u\, G(q)$

The Hamiltonian: $H(q,u,p) = H_F(q,p) + u\, H_G(q,p), \; H_i = < p, F_i >, \; i = F, G$

$\Rightarrow$ The singular extremals are those contained in $H_G = 0$.

[BCG+11] B. Bonnard, O. Cots, S. Glaser, M. Lapert, and D. Sugny.
Geometric optimal control of the contrast imaging problem in nuclear magnetic resonance.
math.u-bourgogne.fr, 2011.

Single spin: singular extremals

$\Rightarrow$ The singular extremals are those contained in $H_G = 0$.

$$\left.\begin{array}{rclcl} H_G &=& <p,G> &=& 0 \\ \dot{H}_G &=& <p,[G,F]> &=& 0 \end{array}\right\} \Rightarrow \det(G,[G,F]) = y(-2\delta z+\gamma) = 0$$

with $\delta = \gamma - \Gamma$.

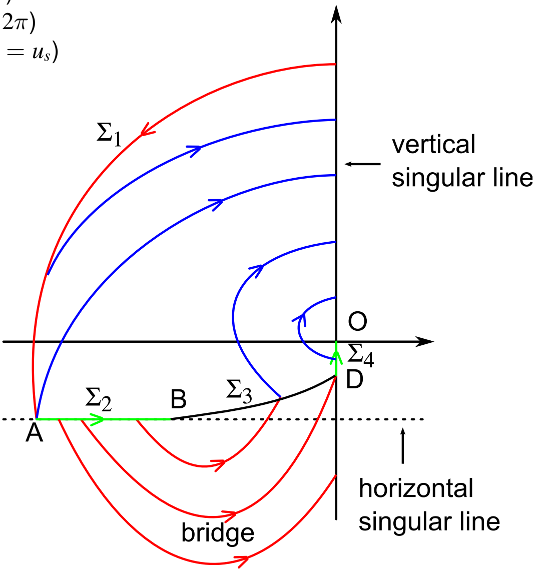
The singular lines are $y = 0$ and $z_0 = \frac{\gamma}{2\delta}$. The singular control $u_s(q,p)$ is computed from $\ddot{H}_G = \{\{H_G, H_F\}, H_F\}(z) + u_s\{\{H_G, H_F\}, H_G\}(z) = 0$.

Horizontal line ($z_0 = \frac{\gamma}{2\delta}$): optimal, according to Generalized Legendre-Clebsch condition (see [BC03]) and $u_s(q) = \gamma(2\Gamma-\gamma)/(2\delta y) \Rightarrow u_s \in L^1$, $u_s \notin L^2$

Vertical line ($y = 0$): optimal for $z_0 < z < 1$ (GLC) and $u_s(q) = 0$.

[BC03] B. Bonnard and M. Chyba.
Singular trajectories and their role in control theory, mathématiques & applications, vol. 40.
lavoisier.fr, Jan 2003.

Red: bang ($u = 2\pi$)
Blue: bang ($u = -2\pi$)
Green: singular ($u = u_s$)
B: saturation



Summary: single spin => contrast problem

- Solutions of the contrast problem are made of Bang-Singular sequences.
- We get T_{min}.
- The solution for the limit case $t_f = T_{min}$ is B^+SB^+S.

To solve the contrast problem, we use an indirect method (multiple shooting)

$\Rightarrow$ we need to know the structure a priori.

$\Rightarrow$ we use an homotopic approach to capture the structure and initialize the multiple shooting method.

$$
(P_\lambda)\begin{cases}
-\left(y_2^2(t_f)+z_2^2(t_f)\right)+(1-\lambda)\int_0^{t_f}|u|^{2-\lambda}(t)dt \to \min \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad q_i=(y_i,z_i),\ |q_i|\le 1,\ i=1,2 \\
\left[\begin{array}{lllll} \dot{y}_1 & = & -\Gamma_1\, y_1 & - & u\, z_1 \\ \dot{z}_1 & = & \gamma_1(1-z_1) & + & u\, y_1 \end{array}\right. \qquad \gamma_i=1/(32.3\ T_{i1}) \\
\left[\begin{array}{lllll} \dot{y}_2 & = & -\Gamma_2\, y_2 & - & u\, z_2 \\ \dot{z}_2 & = & \gamma_2(1-z_2) & + & u\, y_2 \end{array}\right. \qquad \Gamma_i=1/(32.3\ T_{i2}) \\
\qquad\qquad\qquad\qquad\qquad\qquad\qquad\qquad |u|\le 2\pi \\
q_1(0)=(0,1)=q_2(0) \\
q_1(t_f)=(0,0)
\end{cases}
$$

Homotopy (P_λ): $-\left(y_2^2(t_f)+z_2^2(t_f)\right)+(1-\lambda)\int_0^{t_f}|u|^{2-\lambda}(t)dt \to \min$

The Hamiltonian: $H(q,u,p,\lambda)=H_F(q,p)+u\,H_G(q,p)+(1-\lambda)\,|u|^{2-\lambda}$

(P_λ)-extremals are admissible for (P).

Maximum principle

The maximization of the Hamiltonian gives:

$$u(q,p,\lambda) = \underset{w \in U}{argmax} \quad H(q,w,p,\lambda)$$

and we have

$$\lambda < 1 \Rightarrow u = sign(H_G) \min \left(2\pi, \left(\frac{2|H_G|}{((2-\lambda)(1-\lambda))} \right)^{\frac{1}{(1-\lambda)}} \right)$$

We call true Hamiltonian the function (which does not depend on u)

$$H_r(q,p,\lambda) = H(q,u(q,p,\lambda),p,\lambda)$$

In order to solve the problem (P) in $\lambda = 1$, we:

1. solve by simple shooting method the problem in $\lambda = 0$ easily,
2. use homotopic method to solve (P_λ), from $\lambda = 0$ to $\lambda = \lambda_f < 1$, to ...
3. ... capture the structure of (P) and initialize the multiple shooting method.

Smooth optimal control problem (P_λ)

↓ (PMP)

$$(BVP_\lambda)\begin{cases}(\dot{x},\dot{p}) = \vec{H}(x,p,\lambda) = \left(\frac{\partial H(x,p,\lambda)}{\partial p}, -\frac{\partial H(x,p,\lambda)}{\partial x}\right)\\ b_0(x(0),p(0),\lambda) = 0 \in \mathbb{R}^n\\ b_f(x(t_f),p(t_f),\lambda) = 0 \in \mathbb{R}^n\end{cases}$$

↓ (Shooting method)

$$S_\lambda(x_0,p_0) = \begin{pmatrix} b_0(x_0,p_0,\lambda)\\ b_f(x_f,p_f,\lambda)\end{pmatrix} = 0 \ (S : \mathbb{R}^{2n} \to \mathbb{R}^{2n})$$

with $(x_f,p_f) \equiv (x(t_f,x_0,p_0,\lambda), p(t_f,x_0,p_0,\lambda)) = exp_{t_f}\vec{H}(x_0,p_0,\lambda)$

The final time t_f is equal to $1.1T_{min}$ where T_{min} is the minimal time to transfer the spin 1 from $(0,1)$ to $(0,0)$.

Blood case:
Spin 1 = (De)oxygenate blood : $T_{11} = 1350$ and $T_{21} = 200$
Spin 2 = Oxygenate blood : $T_{12} = 1350$ and $T_{22} = 50$

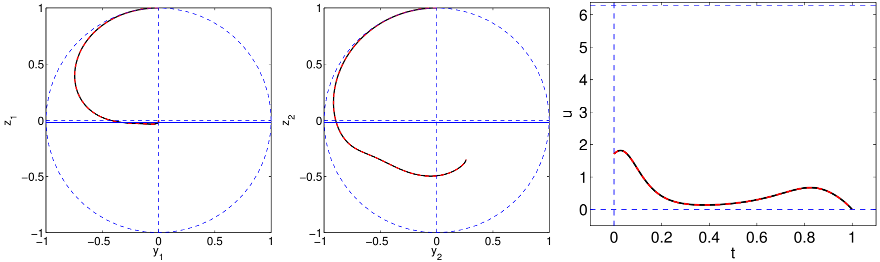


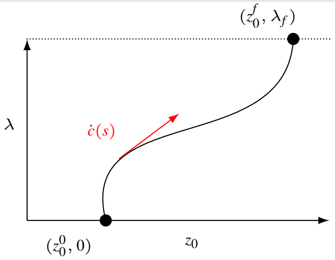
Figure: Solution for $\lambda = 0$ with $L^{2-\lambda}$ regularization. Trajectories of spin 1 and 2 and the control associated.

Let us define the homotopic function

$$\begin{array}{rcl} h : \mathbb{R}^{2n} \times [0,1] & \longrightarrow & \mathbb{R}^{2n} \\ (z_0, \lambda) & \longmapsto & S_\lambda(z_0) \end{array}$$

with $z_0 = (q_0, p_0)$.
Assuming that 0 is a regular value for h, the level set $\{h = 0\}$ is a one dimensional submanifold of $\mathbb{R}^{2n+1}$ called the path of zeros.

We know a zero of $h(., \lambda)$ for $\lambda_0 = 0$ noted z_0^0, and we want to follow this path to reach a zero for a target value of the parameter λ close to 1.



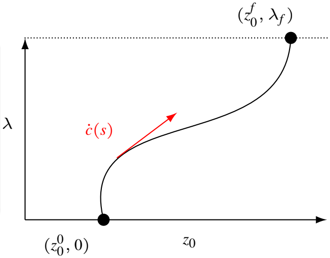
HAMPATH uses DOPRI5 from E. Hairer and G. Wanner [HrW93] [HW], for the numerical integration (without any correction) of:

$$(IVP) \begin{cases} \dot{c}(s) = T(c(s)) \\ c(0) = (z_0^0, 0) \end{cases}$$

Until s_f such that $\lambda(s_f)$ close to 1 (dense output).

$\dot{c}(s) = T(c(s))$ is determined by

1. $h'(c(s))\dot{c}(s) = 0$
2. $|\dot{c}(s)|$=1
3. $\det \begin{pmatrix} h'(c(s)) \\ {}^t\dot{c}(s) \end{pmatrix}$ is of constant sign



[HrW93] E. Hairer, S.P. Nørsett, and G. Wanner.
Solving Ordinary Differential Equations I, Nonstiff Problems, volume 8 of *Springer Serie in Computational Mathematics*.
Springer-Verlag, second edition, 1993.

[HW] E. Hairer and G. Wanner.
DOPRI5 `http://www.unige.ch/~hairer/prog/nonstiff/dopri5.f`.

The path of zeros: $\lambda_f = 0.915$: Blood case

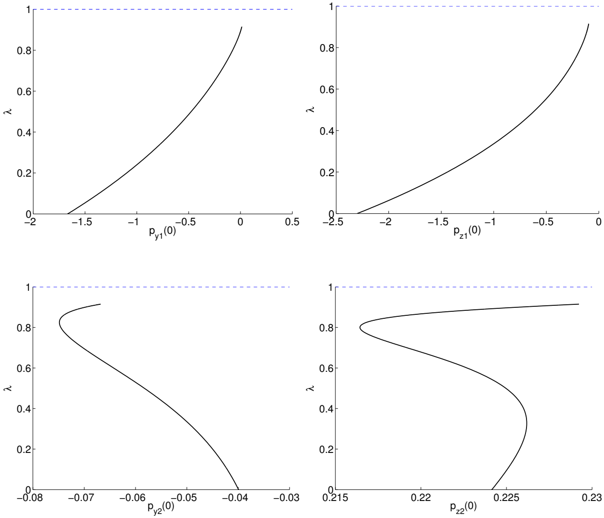
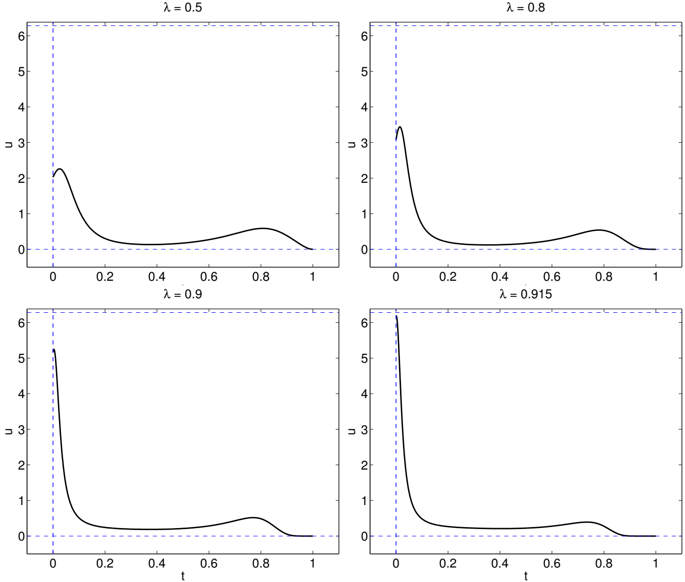
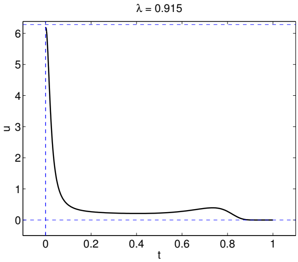


Figure: Homotopic path with $L^{2-\lambda}$ regularization. Initial adjoint vector w.r.t. λ.

Control: $\lambda \in \{0.5, 0.8, 0.9, 0.915\}$: Blood case



States-Control: $\lambda = 0.915$: Blood case



$\longrightarrow$ Bang-Singular structure.

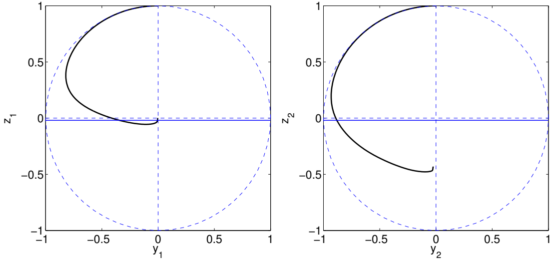


Figure: Solution for $\lambda = 0.915$ with $L^{2-\lambda}$ regularization. Trajectories of spin 1 and 2 and the control associated.

We have a BS structure for $t_f = 1.1T_{min}$. We denote by t_0, t_1, t_f the different instants and by z_0, z_1, z_f the the associated state and costate variables ($z = (q_1, q_2, p_1, p_2) \in \mathbb{R}^4 \times \mathbb{R}^4$).

- Hamiltonian :

$$H(q,u,p) = H_F(q,p) + u\, H_G(q,p), \begin{cases} u = 2\pi & \text{if } t \in [t_0; t_1] \\ u = u_{sing} & \text{if } t \in [t_1; t_f] \end{cases}$$

- Equations (*cf.* [Mau76]) :

$$\begin{array}{ccccc} & \textit{Bang} & & \textit{Sing} & \\ (t_0, z_0) & \longrightarrow & (t_1, z_1) & \longrightarrow & (t_f, z_f) \\ q_1 = (0,1) & & H_G = 0 & & q_1 = (0,0) \\ q_2 = (0,1) & & \dot{H}_G = 0 & & q_2 = p_2 \end{array}$$

with the matching conditions $z(t_1; t_0, z_0) = z_1$.

[Mau76] H. Maurer.
Numerical solution of singular control problems using multiple shooting techniques.
Journal of optimization theory and applications, Jan 1976.

We used the solution at $\lambda = 0.915$ to initialise the multiple shooting. The time t_1 is taken in $[0.01, 0.2]$ and leads to the following solutions.

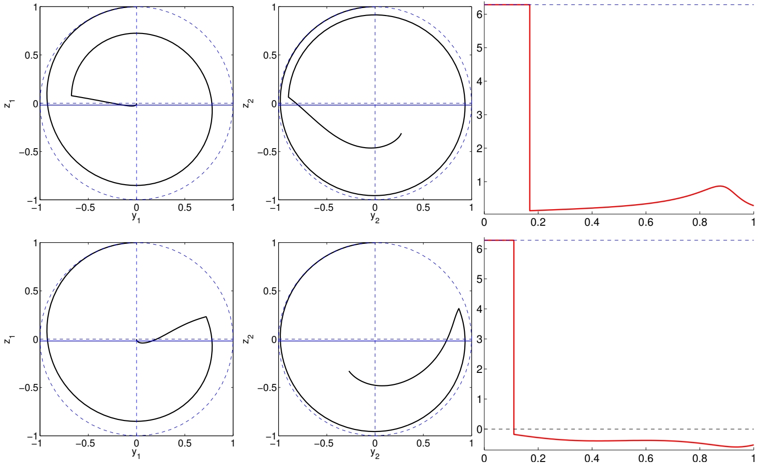


Figure: (TOP) First solution (contrast of 0.41). (BOTTOM) Second solution (contrast of 0.42). From the $L^{2-\lambda}$ regularization.

Trajectories of spin 1 and 2 and the control: blood case $(\lambda = 1.0)$

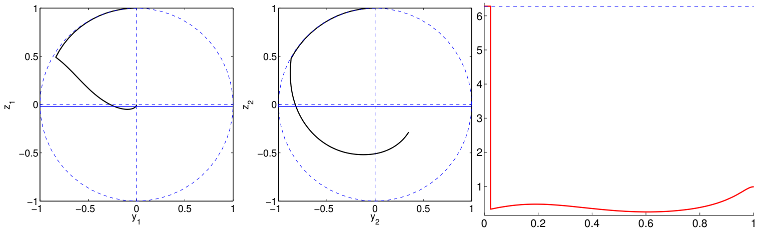


Figure: Best solution (contrast of 0.45) from the $L^{2-\lambda}$ regularization.

Summary

- The regularizations $L^{2-\lambda}$ permit to find solutions satisfying the first order necessary conditions of optimality and BS structure has been detected.
- To solve in $\lambda = 0$ is very easy.
- Homotopy is automatic: we do not need to provide any steps grid.
- But there are many local solutions.

Contrast problem: sensitivity w.r.t. the final time t_f

We use HAMPATH to perform a differential continuation on t_f between $T_{min} + \varepsilon$ and $2T_{min}$.

- T_{min} : the minimal time to transfer the spin 1 from $(0, 1)$ to $(0, 0)$.

$\hookrightarrow$ there is an horizontal asymptote on the contrast plot. 99% of the optimal solution is obtained for $t_f = 1.3T_{min}$.

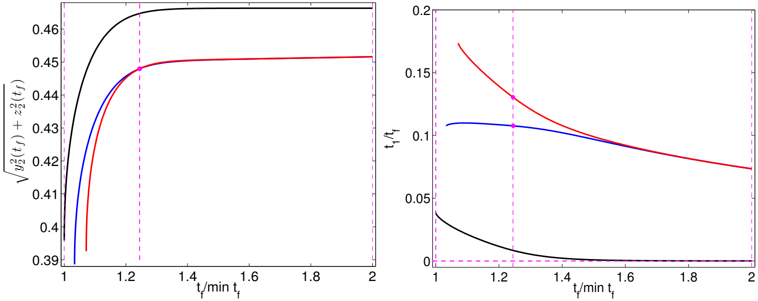


Figure: Best solution in black. (LHS) Contrast w.r.t the transfer duration. (RHS) Normalized switching time.

Solution for the limit case: t_f close to T_{min}

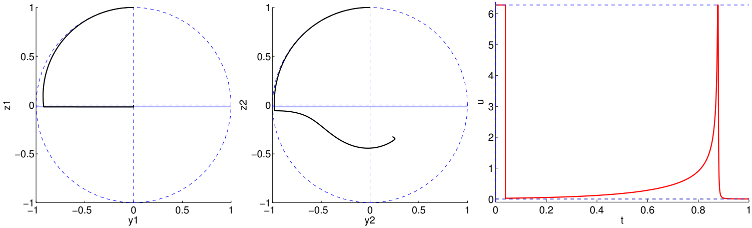


Figure: Best solution for $t_f = 1.000004 \times \min t_f$.

The final time t_f is equal to $1.5T_{min}$ where T_{min} is the minimal time to transfer the spin 1 from $(0,1)$ to $(0,0)$.

Fluid case:
Spin 1 = Cerebrospinal fluid : $T_{11} = 2000$ and $T_{21} = 200$
Spin 2 = Water : $T_{12} = 2500$ and $T_{22} = 2500$

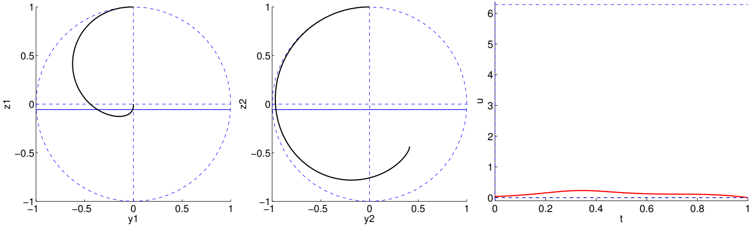


Figure: Solution for $\lambda = 0$ with $L^{2-\lambda}$ regularization. Trajectories of spin 1 and 2 and the control associated.

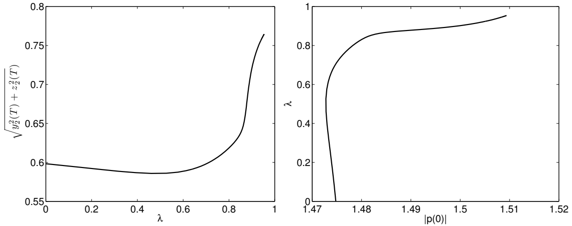


Figure: $\lambda = 0.0 \rightarrow \lambda = 0.954$, contrast $\in [0.586, 0.765]$ and norm of the path.

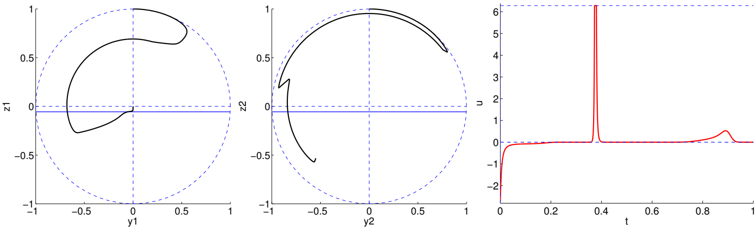


Figure: Solution for $\lambda = 0.954$ (contrast of 0.765) from the $L^{2-\lambda}$ regularization.

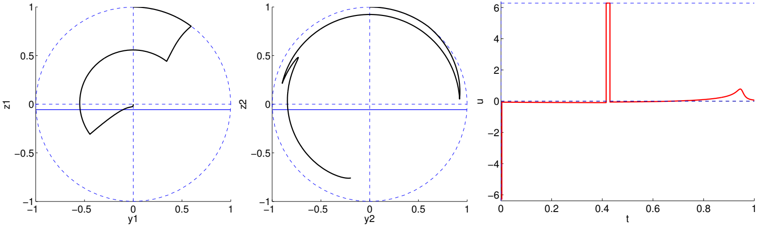


Figure: Solution for $\lambda = 1$, $t_f = 1.5T_{min}$ (contrast of 0.783) from the $L^{2-\lambda}$ regularization.

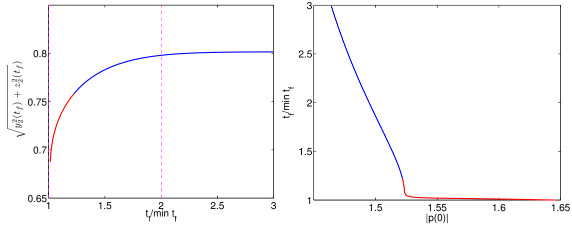


Figure: (BLUE) 2-BS structure. (RED) 3-BS structure. Homotopy: $t_f = 3T_{min} \to t_f = T_{min}$, contrast $\in [0.69, 0.8]$ and norm of the path.

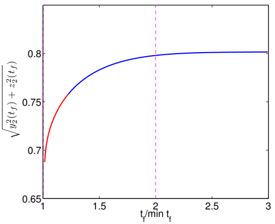


Figure: (BLUE) 2-BS structure. (RED) 3-BS structure. Contrast w.r.t. t_f.

During the continuation we detect that for $t_f = 1.225T_{min}$, the last singular control does not respect the constraint ($u_s <= 2\pi$). Hence, we add a Bang arc, which consists in adding two switching times in the multiple shooting formulation and we have a $3BS$-structure.

New results in the blood case: homotopy on parameters

Spin 1 (y_1, z_1) -	Deoxygenated blood	: $T_{11} = 1350$ ms,	$T_{12} = 50$	ms
Spin 2 (y_2, z_2) -	Oxygenated blood	: $T_{21} = 1350$ ms,	$T_{22} = 200$	ms
Spin 1 (y_1, z_1) -	Cerebrospinal fluid	: $T_{11} = 2000$ ms,	$T_{12} = 200$	ms
Spin 2 (y_2, z_2) -	Water	: $T_{21} = 2500$ ms,	$T_{22} = 2500$	ms

We perform here a continuation on the physical parameters from the Fluid case to the Blood one.

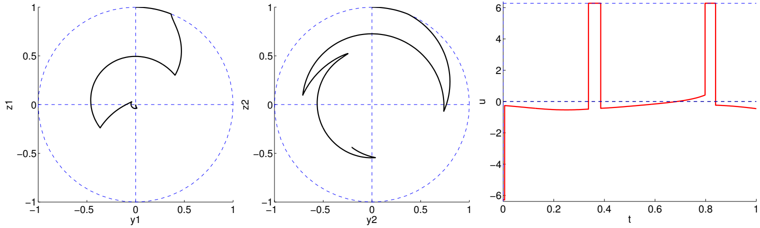


Figure: $3BS$ solution for the blood case, obtained from the $2BS$ fluid solution. Here $\lambda = 1.0$, $t_f = 1.5T_{min}$, contrast is 0.484.

New results in the blood case: homotopy on the final time

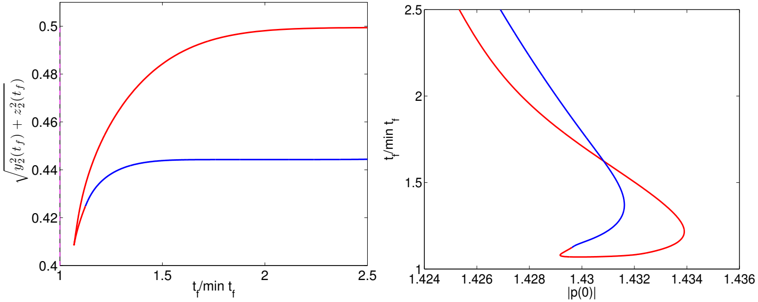


Figure: (BLUE) $2BS$-structure. (RED) $3BS$-structure. Contrast and norm of the path w.r.t. t_f

Old and New results in the blood case

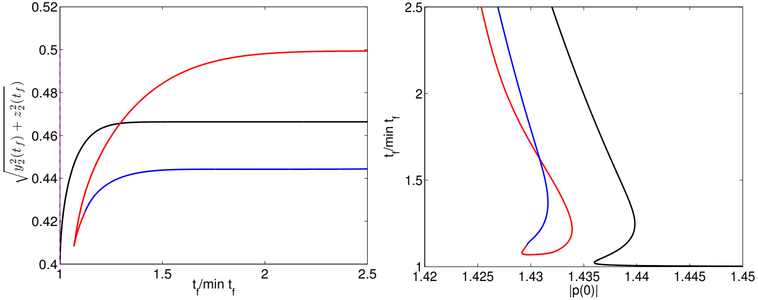


Figure: (BLACK) BS-structure. (BLUE) $2BS$-structure. (RED) $3BS$-structure. Contrast and norm of the path w.r.t. t_f

⇒ The optimal structure varies according to t_f which is not detected in this case, during the path following.

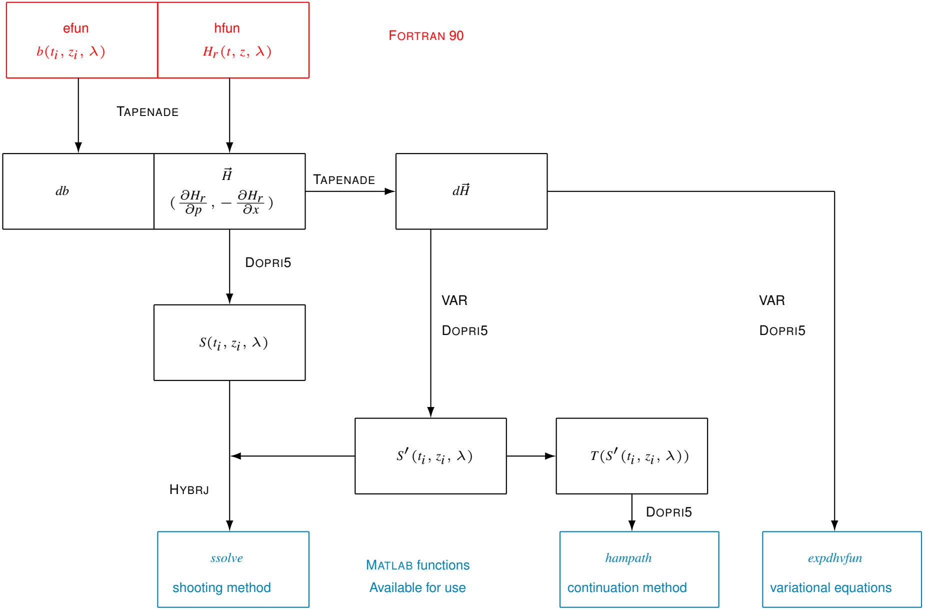
From the true hamiltonian and the boundary, intermediate and transversality conditions, HAMPATH [CCG11]:

- produces automatically the state-costate equations (thanks to TAPENADE)
- computes the shooting function by numerical integration (thanks to DOPRI5)
- provides the variational equations used in the jacobian of the shooting function (thanks to TAPENADE)
- integrates the variational equations so that the diagram commutes (the step size control is only made on the state and co-state equations)

$$\begin{array}{ccc} (IVP) & \xrightarrow{\text{Numerical integration}} & h(z_0, \lambda) \\ \text{Derivative} \downarrow & & \downarrow \text{Derivative} \\ (VAR) & \xrightarrow{\text{Numerical integration}} & \frac{\partial h}{\partial z_0}(z_0, \lambda) \end{array}$$

[CCG11] J.B. Caillau, O. Cots, and J. Gergaud.
Differential pathfollowing for regular optimal control problems. HAMPATH apo.enseeiht.fr/hampath.
Optimization Methods and Software, to appear, 2011.

Global diagram of HAMPATH



Conclusion

- The HAMPATH package [CCG11] gives tools to solve OCP by indirect methods:
  - Shooting methods: simple and multiple;
  - Homotopic methods: differential without correction;
  - Function which integrate the variationnal equations and permit to check sufficient second order conditions in the smooth case;
  - ...
- The derivatives and the functions are computed accurately and automatically.
- It is very easy to use since only 2 FORTRAN subroutines need to be implemented. Then it is interfaced with MATLAB.

- Homotopic method detects BS and $2BS$-structures and gives good initial points for multiple shooting.
- It gives also some sensitivity w.r.t to the final time and parameters.
- Finding the global optimum is stil an open problem.
- Some work have been done about second order conditions for the contrast problem with BS structure (see [BC12] for details);

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