On solving optimal control problems by continuation and multiple shooting methods

15th Austrian-French-German conference on Optimization

O. Cots

AFG’11, Toulouse, September 19-23, 2011
Introduction - Collaborations

-- Bernard Bonnard (Univ. Bourgogne)
-- Jean-Baptiste Caillau (Univ. Bourgogne)
-- Joseph Gergaud (N7 - IRIT)
-- Steffen J. Glaser (Univ. Munich)
-- Dominique Sugny (Univ. Bourgogne)
-- ...

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

\[
|q_2(t_f)|^2 = (y_2^2(t_f) + z_2^2(t_f)) \rightarrow \max
\]

\[
\begin{align*}
\dot{y}_1 &= -\Gamma_1 y_1 - u z_1 \\
\dot{z}_1 &= \gamma_1 (1 - z_1) + u y_1 \\
\dot{y}_2 &= -\Gamma_2 y_2 - u z_2 \\
\dot{z}_2 &= \gamma_2 (1 - z_2) + u y_2
\end{align*}
\]

\[
q_1(0) = (0, 1) = q_2(0) \\
q_1(t_f) = (0, 0)
\]

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

\[
\gamma_i = 1/(32.3 \ T_{i1}) \\
\Gamma_i = 1/(32.3 \ T_{i2})
\]

\[
|u| \leq 2\pi
\]

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

\[ (P_1) \begin{cases}
  t_f \to \min \\
  \dot{y} = -\Gamma y - u z \\
  \dot{z} = \gamma(1 - z) + u y \\
  q(0) = (0, 1) \\
  q(t_f) = (0, 0)
\end{cases} \]

\[ q = (y, z), \ |q| \leq 1 \]

\[ \frac{3\gamma}{2} < \Gamma \]

\[ |u| \leq 2\pi \]

The dynamics:
\[ \dot{q} = F(q) + u G(q) \]

The Hamiltonian:
\[ H(q, u, p) = H_F(q, p) + u H_G(q, p), \ H_i = \langle p, F_i \rangle, \ i = F, G \]

⇒ The singular extremals are those contained in \( H_G = 0 \).
The singular extremals are those contained in $H_G = 0$.

\[
\begin{align*}
H_G &= \langle p, G \rangle = 0 \\
\dot{H}_G &= \langle p, [G, F] \rangle = 0
\end{align*}
\] \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 $u_s(q) = 0$. 
Single spin : global synthesis

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

Results on contrast problem

O. Cots (IMB Bourgogne)
Single spin $\Rightarrow$ contrast problem

- We need to start with a bang.

- Singular extremals are expected for the contrast problem.

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.
Homotopy $(P_\lambda)$:

\[
\begin{aligned}
(-y_2^2(t_f) + z_2^2(t_f)) + (1 - \lambda) \int_0^{t_f} |u|^{2-\lambda} \, dt \to \min \\

\begin{cases}
\dot{y}_1 &= - \Gamma_1 y_1 - u z_1 \\
\dot{z}_1 &= \gamma_1 (1 - z_1) + u y_1 \\
\dot{y}_2 &= - \Gamma_2 y_2 - u z_2 \\
\dot{z}_2 &= \gamma_2 (1 - z_2) + u y_2 \\
q_1(0) &= (0, 1) = q_2(0) \\
q_1(t_f) &= (0, 0)
\end{cases}
\end{aligned}
\]

\[\gamma_i = 1/(32.3 \, T_{i1}) \quad \Gamma_i = 1/(32.3 \, T_{i2}) \quad |u| \leq 2\pi\]

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

$(P_\lambda)$-extremals are admissible for $(P)$.
The maximization of the Hamiltonian gives:

\[ u(q, p, \lambda) = \arg\max_{w \in U} H(q, w, p, \lambda) \]

and we have

\[ \lambda < 1 \Rightarrow \begin{cases} 
  u = \text{sign}(H_G) \cdot \left\{ \frac{2|H_G|}{((2-\lambda)(1-\lambda))} \right\}^{\frac{1}{(1-\lambda)}} & \text{if } |u| \leq 2\pi \\
  u = 2\pi \cdot \text{sign}(H_G) & \text{else}
\end{cases} \]

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 \((P_{\lambda})\), from \(\lambda = 0\) to \(\lambda = \lambda_f < 1\), to . . .
3. . . . capture the structure of \((P)\) and initialize the multiple shooting method.
1 : Solving in $\lambda = 0$ with simple shooting method

The final time $t_f$ is equal to $1.1T_{\text{min}}$ where $T_{\text{min}}$ 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 define the homotopic function

\[ h : \mathbb{R}^{2n} \times [0, 1] \rightarrow \mathbb{R}^{2n} \]

\[ (z_0, \lambda) \mapsto S_\lambda(z_0) \]

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 \( \lambda \) close to 1.
**Differential algorithms**

**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 as \( \lambda(s_f) \) close to 1 (dense output).

Under generic assumptions, \( \dot{c}(s) = T(c(s)) \) is determined by:

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

---


The path of zeros: $\lambda_f = 0.915$.

**Figure:** Homotopic path with $L^2-\lambda$ regularization. Initial adjoint vector w.r.t. $\lambda$. 
Control: $\lambda \in \{0.5, 0.8, 0.9, 0.915\}$
States-Control : $\lambda = 0.915$

$\lambda = 0.915$

$\lambda = 0.915$

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

- **Hamiltonian**: 
  \[
  H(q, u, p) = H_F(q, p) + u \ H_G(q, p), \quad \left\{
  \begin{array}{ll}
  u = 2\pi & \text{if } t \in [t_0; t_1] \\
  u = u_{\text{sing}} & \text{if } t \in [t_1; t_f]
  \end{array}
  \right.
  \]

- **Equations (cf. [Mau76])**: 
  
  \[
  \begin{align*}
  (t_0, z_0) & \quad \rightarrow \quad (t_1, z_1) & (t_f, z_f) \\
  q_1 & = (0, 1) & H_G & = 0 & q_1 & = (0, 0) \\
  q_2 & = (0, 1) & \dot{H}_G & = 0 & q_2 & = p_2
  \end{align*}
  \]

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

**Figure:** First solution (contrast of 0.41) from the $L^2-\lambda$ regularization.

**Figure:** Second solution (contrast of 0.42) from the $L^2-\lambda$ regularization.
The limitation of the $L^2-\lambda$ regularization.

Let define the $L^2$ regularization:

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

The Hamiltonian becomes:

$$H(q, u, p, \lambda) = H_F(q, p) + u H_G(q, p) + (1 - \lambda) |u|^2$$

And the maximization of the $H$ gives:

$$\lambda < 1 \Rightarrow \begin{cases} 
  u = -\frac{H_G}{2(1-\lambda)p^0} & \text{if } |u| \leq 2\pi \\
  u = 2\pi \text{sign}(H_G) & \text{else}
\end{cases}$$

We find a better solution with contrast about 0.45. The two previous solutions are just local optimums.

**Figure:** Best solution (contrast of 0.45) from the $L^2$ regularization.
We have an optimal control problem with Bang and Singular arcs. The regularizations $L^{2-\lambda}$ and $L^2$ permit to find solutions satisfying the first order necessary conditions of optimality.

To solve in $\lambda = 0$ is very easy.

$L^{2-\lambda}$ captures the BS structure very well compared to $L^2$. However we only get the best solution with $L^2$. 

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

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

$\rightarrow$ there is an horizontal asymptote on the contrast plot. The optimal solution in terms of contrast is obtain from $t_f = 1.3T_{\text{min}}$.

**Figure**: (LHS) Contrast w.r.t the transfer duration. (RHS) Normalized duration of the Bang arc.
From the true hamiltonian and the boundary, intermediate and transversality conditions, HAMPATH [CCG11] :

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

\[
\begin{align*}
(IVP) & \quad \text{Numerical integration} \quad h(z_0, \lambda) \\
\text{Derivative} & \quad \downarrow \qquad \downarrow \text{Derivative} \\
(VAR) & \quad \text{Numerical integration} \quad \frac{\partial h}{\partial z_0}(z_0, \lambda)
\end{align*}
\]
Global diagram of HAMPATH

\[ \text{efun} \quad b(t_i, z_i, \lambda) \]

\[ \text{hfun} \quad H_R(t, z, \lambda) \]

\[ \frac{\partial H_R}{\partial p}, -\frac{\partial H_R}{\partial x} \]

\[ \overrightarrow{H} \]

\[ d\overrightarrow{H} \]

\[ S(t_i, z_i, \lambda) \]

\[ S'(t_i, z_i, \lambda) \]

\[ T(S'(t_i, z_i, \lambda)) \]

**FORTRAN 90**

**TAPENADE**

**DOPRI5**

**MATLAB functions**

Available for use

**hampath**

continuation method

**expdhvfun**

variational equations

**ssolve**

shooting method

**HYBRJ**

**O. Cots (IMB Bourgogne)**

Results on contrast problem

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The HAMPATH package gives tools to solve OCP by indirect methods:

- Shooting methods: simple and multiple;
- Homotopic methods: differential without correction and discrete;
- Function which integrates 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 gave us the right structure and a good initial point for the contrast problem. We could compute the solution with accuracy thanks to multiple shooting.

Work in progress:

- Second order conditions for regularized problem and BS structure;
- Convergence of the zeros path to the best solution.
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H. Maurer. 