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# Differential continuation for regular optimal control problems 

J.-B. Caillau ${ }^{\text {a }}$, O. Cots ${ }^{\text {a }}$ and J. Gergaud ${ }^{\text {b }}$<br>${ }^{a}$ Math. Institute, Bourgogne Univ. \& CNRS, 2 avenue Savary, F-21078 Dijon, France; ${ }^{b}$ ENSEEIHT-IRIT, Toulouse Univ. \& CNRS, 2 rue Camichel, F-31071 Toulouse, France


#### Abstract

Regular control problems in the sense of the Legendre condition are defined, and second-order necessary and sufficient optimality conditions in this class are reviewed. Adding a scalar homotopy parameter, differential pathfollowing is introduced. The previous sufficient conditions ensure the definiteness and regularity of the path. The role of AD for the implementation of this approach is discussed, and two examples excerpted from quantum and space mechanics are detailed.


Keywords: optimal control; second-order conditions; conjugate points; differential homotopy; automatic differentiation

AMS Subject Classification: 49K15; 49-04

## 1. Introduction

In [15], automatic differentiation allowed to assemble the two-point boundary value problem embodying the first-order necessary optimality condition of an optimal control problem. ADIFOR [6] was used, and sensitivities were computed using automatic differentiation (AD) again, in connection with primitive second-order optimality conditions. This approach was given a full treatment with the development of the cotcot code [11]. Given the data defining the control problem, a set of Matlab routines was generated through AD so as to solve the problem by single shooting and to systematically check conjugate point second-order conditions [9]. This paper aims at presenting the next step, that is the addition of a layer automating differential pathfollowing for optimal control problems depending on one scalar homotopic parameter: The differential equation that embodies the continuation procedure is automatically generated and numerical integration performed. The resulting code [17] relies crucially on AD to compile the definition of the parametric control problem into a collection of Matlab Mex-files. In particular, the core of the method is to replace shooting by the mere integration of an AD-defined ordinary differential equation (ODE). Differential pathfollowing replaces Newton solving - except for the computation of the starting point where shooting is still needed - , and provides numerical checks all along the path of optimal control second-order sufficient conditions.

[^0]The paper is organized in five sections. The first one settles the mathematical framework for second-order necessary and sufficient conditions. The infinite-dimensional setting together with the dynamical features typical of optimal control of ODEs have some peculiarities, and we give a more or less self-contained overview of the necessary part along the lines of [1]. Section 2 introduces differential homotopy for the regular class of optimal control problems just defined. The role of AD and other algorithmic issues are reviewed in Section 3. Finally, two examples coming from ongoing research projects are treated. One in dissipative quantum control, the other in space mechanics. In the first case, homotopy explores the change of solutions in a range of physical parameters, while in the latter pathfollowing is used to regularize and simplify the $\mathrm{L}^{1}$-minimization problem considered.

## 2. Second-order conditions for regular optimal control problems

Let us consider the following optimal control problem: Minimize the integral or Lagrange cost functional

$$
\int_{0}^{t_{f}} f^{0}(x(t), u(t)) \mathrm{d} t \longrightarrow \min
$$

subject to differential constraints

$$
\dot{x}(t)=f(x(t), u(t)), \quad u(t) \in U, \quad t \in\left[0, t_{\mathrm{f}}\right]
$$

and boundary conditions

$$
x(0)=x_{0}, \quad x\left(t_{\mathrm{f}}\right)=x_{\mathrm{f}} .
$$

The state, $x$, lives on an $n$-dimensional manifold ${ }^{1} X$ so, in local coordinates, $x(t) \in \mathbf{R}^{n}$. The control, $u$, belongs to an $m$-dimensional manifold $U$. Being without a boundary, $U$ has charts with open domains in $\mathbf{R}^{m}$ and $u(t) \in \mathbf{R}^{m}$, locally. The latter is a strong restriction as typical control problems involve control constraints, that is manifolds $U$ with a boundary. ${ }^{2}$ Such an example is addressed in Section 6. For the sake of simplicity, the positive final time $t_{\mathrm{f}}$ is assumed to be fixed. The data $\left(f^{0}, f\right)$ is smooth ${ }^{3}$ in $(x, u)$. We seek a measurable, essentially bounded control so, in coordinates, $u \in \mathrm{~L}_{m}^{\infty}\left(\left[0, t_{\mathrm{f}}\right]\right)=\mathrm{L}^{\infty}\left(\left[0, t_{\mathrm{f}}\right], \mathbf{R}^{m}\right)$. In order to assess the first- and second-order necessary optimality conditions, let $\bar{u}$ be an optimal control, and let $\bar{x}$ be the associated Lipschitz optimal trajectory defined on the whole interval $\left[0, t_{\mathrm{f}}\right]$. We define the augmented system, which amounts to incorporating the cost into the state. Set $\hat{x}=\left(x^{0}, x\right) \in \mathbf{R}^{n+1}$. Almost for all $t$,

$$
\dot{\hat{x}}(t)=\hat{f}(\hat{x}(t), u(t)) \quad \text { with } \hat{f}(\hat{x}, u)=\left(f^{0}, f\right)(x, u)
$$

Define $\hat{x}(0)=\left(0, x_{0}\right)$, so the cost is retrieved as one of the components of the augmented state. From now on, we drop the ^ on variables to simplify notation, keeping in mind that in our context $x(t) \in \mathbf{R}^{n}$ stands for $\left(x^{0}(t), x(t)\right) \in \mathbf{R}^{n+1}$, and $f$ for $\left(f^{0}, f\right)$. What follows is a very partial account of [1, Chapter 20-21], without the differential-geometric machinery. Among many others, see also $[8,25,28]$ and references therein.

For any $s \in\left[0, t_{\mathrm{f}}\right]$, the endpoint mapping

$$
F_{\mathrm{s}}: u \longmapsto x(s, u) \in \mathbf{R}^{n}
$$

that maps a control to the solution of

$$
\dot{x}(t)=f(x(t), u(t)), \quad x(0)=x_{0}
$$

is well defined and smooth in a neighbourhood in $L_{m}^{\infty}([0, s])$ of $\bar{u}$ by virtue of the implicit function theorem, and

$$
F_{\mathrm{s}}^{\prime}(\bar{u}) \delta u=\delta x(s), \quad \delta u \in \mathrm{~L}_{m}^{\infty}([0, s]),
$$

where $\delta x$ is the solution of

$$
\begin{equation*}
\delta \dot{x}(t)=\partial_{x} f(\bar{x}(t), \bar{u}(t)) \delta x(t)+\partial_{u} f(\bar{x}(t), \bar{u}(t)) \delta u(t), \quad \delta x(0)=0 . \tag{1}
\end{equation*}
$$

The first order necessary condition is obtained asserting that $F_{t_{\mathrm{f}}}$ cannot be locally open ${ }^{4}$ at $\bar{u}$. We recall the following standard (nonlinear) open mapping result.

Theorem 2.1 Let $F: E \rightarrow \mathbf{R}^{n}$ be a smooth ${ }^{5}$ mapping on the Banach space $E$. Let u be a non-critical point $\left(F^{\prime}(u)\right.$ is onto), then $F$ is locally open at $u$.

As result, $F_{t_{\mathrm{f}}}^{\prime}(\bar{u})$ cannot be onto, and there is a non-zero covector $\lambda \in\left(\mathbf{R}^{n}\right)^{*}$ such that $\bar{\lambda} F_{t_{\mathrm{f}}}^{\prime}(\bar{u})=$ 0 . This is the Lagrange rule which gives Pontryagin maximum principle in a weak form. Let $\bar{p}$ be the Lipschitz solution (valued in $\left.\left(\mathbf{R}^{n}\right)^{*}\right)$ of the adjoint equation

$$
\dot{p}(t)=-p(t) \partial_{x} f(\bar{x}(t), \bar{u}(t)), \quad p\left(t_{\mathrm{f}}\right)=\bar{\lambda} .
$$

The triple $(\bar{x}, \bar{u}, \bar{p})$ is called an extremal. For any $\delta u \in \mathrm{~L}_{m}^{\infty}\left(\left[0, t_{\mathrm{f}}\right]\right)$,

$$
0=\bar{\lambda} F_{t_{\mathrm{f}}}^{\prime}(\bar{u}) \delta u=\bar{p}\left(t_{\mathrm{f}}\right) \delta x\left(t_{\mathrm{f}}\right) .
$$

Integrating by parts,

$$
\int_{0}^{t_{\mathrm{f}}} \partial_{u} H(\bar{x}(t), \bar{u}(t), \bar{p}(t)) \delta u(t) \mathrm{d} t=0,
$$

where $H(x, u, p)=p f(x, u)$ is the Hamiltonian function. Accordingly, $\partial_{u} H(\bar{x}(t), \bar{u}(t), \bar{p}(t))=$ 0 almost everywhere on $\left[0, t_{\mathrm{f}}\right]$. Further optimality conditions are obtained using the following second-order open mapping theorem below.

Theorem 2.2 Let $F: E \rightarrow \mathbf{R}^{n}$ be a smooth mapping on the Banach space E. Let u be a corank one critical point of $F\left(\operatorname{codim} \operatorname{Im} F^{\prime}(u)=1\right)$, and let $0 \neq \lambda \in\left(\mathbf{R}^{n}\right)^{*}$ belong to $\left[\operatorname{Im} F^{\prime}(u)\right]^{\perp}$. If $\lambda F^{\prime \prime}(u)$ is sign-indefinite on $\operatorname{Ker} F^{\prime}(u)$, then $F$ is locally open at $u$.

The bilinear form $\lambda F^{\prime \prime}(u) \in \mathscr{L}(E, \mathscr{L}(E, \mathbf{R})) \simeq \mathscr{L}_{2}(E, E ; \mathbf{R})$ is called the intrinsic secondorder derivative of $F$ and is defined up to a scalar in the corank one case. In our situation, $\bar{\lambda} F_{t_{\mathrm{f}}}^{\prime \prime}(\bar{u})$ has to be sign-semidefinite on $\operatorname{Ker} F_{t_{\mathrm{f}}}^{\prime}(\bar{u})$ for local optimality to hold. Given $s \in\left[0, t_{\mathrm{f}}\right]$, define the symmetric (Schwarz) bilinear form $B_{\mathrm{s}}=\bar{\lambda} F^{\prime \prime}(\bar{u})$. By the implicit function theorem, for $\delta u$ and $\delta v$ in $\left.\mathrm{L}_{m}^{\infty}([0, s])\right]$,

$$
F_{\mathrm{s}}^{\prime \prime}(\bar{u})(\delta u, \delta v)=\delta_{2} x(s)
$$

with

$$
\begin{aligned}
\delta_{2} \dot{x}(t)= & \partial_{x} f[t] \delta_{2} x(t)+\partial_{x x}^{2} f[t](\delta x(t), \delta y(t))+\partial_{x u}^{2} f[t](\delta x(t), \delta v(t)) \\
& +\partial_{u x}^{2} f[t](\delta u(t), \delta y(t))+\partial_{u u}^{2} f[t](\delta u(t), \delta v(t)), \quad \delta_{2} x(0)=0,
\end{aligned}
$$

and $\delta x$ (resp. $\delta y$ ) associated with $\delta u$ (resp. $\delta v$ ) according to (1). The argument $[t]$ in partial derivatives of $f$ stands for $(\bar{x}(t), \bar{u}(t))$ for notational convenience. Integrating by parts as before,

$$
\begin{aligned}
B_{\mathrm{s}}(\delta u, \delta v)= & \int_{0}^{s}\left[\partial_{x x}^{2} H[t](\delta x(t), \delta y(t))+\partial_{x u}^{2} H[t](\delta x(t), \delta v(t))\right. \\
& \left.+\partial_{u x}^{2} H[t](\delta u(t), \delta y(t))+\partial_{u u}^{2} H[t](\delta u(t), \delta v(t))\right] \mathrm{d} t
\end{aligned}
$$

the argument $[t]$ standing now for $(\bar{x}(t), \bar{u}(t), \bar{p}(t))$. Since $\bar{u}$ is essentially bounded, $B_{\mathrm{s}}$ remains continuous on $\mathrm{L}_{m}^{\infty}([0, s])$ endowed with the weaker $\mathrm{L}^{2}$-norm, ${ }^{6}$ and can be continuously extended to $\mathrm{L}_{m}^{2}([0, s])$ by density. We set

$$
K_{\mathrm{s}}=\overline{\operatorname{Ker} F_{\mathrm{s}}^{\prime}(\bar{u})^{\|}}{ }^{\|\cdot\|_{2}},
$$

and remark that the sign-definiteness of $B_{\mathrm{s}}$ on $\operatorname{Ker} F_{\mathrm{s}}^{\prime}(\bar{u})$ is equivalent to the sign-semidefiniteness on $K_{\mathrm{s}}$ of the extension of $B_{\mathrm{s}}$ to $\mathrm{L}_{m}^{2}$. Using the embedding of the original space into a Hilbert one to check sign-definiteness is referred to as two-norm discrepancy [25]. On this Hilbert space, $B_{\mathrm{s}} \in$ $\mathscr{L}\left(\mathrm{L}_{m}^{2}, \mathscr{L}\left(\mathrm{~L}_{m}^{2}, \mathbf{R}\right)\right) \simeq \mathscr{L}\left(\mathrm{L}_{m}^{2}\right)$ is identified with a self-adjoint operator. Similarly, the restriction $B_{\mathrm{s} \mid K_{\mathrm{s}}}$ of the bilinear form to $K_{\mathrm{s}}$ is identified with $j_{K_{\mathrm{s}}}^{*} B_{\mathrm{s}} j_{K_{\mathrm{s}}} \in \mathscr{L}\left(K_{\mathrm{s}}\right)$ where $j_{K_{\mathrm{s}}}$ is the canonical injection $K_{\mathrm{s}} \hookrightarrow \mathrm{L}_{m}^{2}([0, s])$ (and $j_{K_{\mathrm{s}}}^{*}$ its adjoint). The following assumption, known as the (strong) Legendre condition, will ensure the negative definiteness of $B_{\mathrm{s}}$ on all $\mathrm{L}_{m}^{2}([0, s])$ for small enough $s$ :

$$
\nabla_{u u}^{2} H(\bar{x}(t), \bar{u}(t), \bar{p}(t)) \leq-\alpha I_{m}, \quad t \in\left[0, t_{\mathrm{f}}\right],
$$

for some $\alpha>0$. Extremals verifying the Legendre condition are called regular.
Proposition 2.3 Under the Legendre condition, $B_{\mathrm{s}}$ is identified with the Fredholm operator $\left(-I+R_{\mathrm{s}}\right)$ on $\mathrm{L}_{m}^{2}([0, s]), R_{\mathrm{S}}$ a compact operator, and is negative definite for small $s$.

Proof The Legendre condition implies that

$$
-\int_{0}^{s} \partial_{u u}^{2} H[t](\delta u(t), \delta v(t)) \mathrm{d} t
$$

is an equivalent scalar product on $\mathrm{L}_{m}^{2}([0, s])$. In this identification, $B_{\mathrm{s}}=-I+R_{\mathrm{S}}$ where $R_{\mathrm{S}}$ is associated with the bilinear part

$$
\begin{equation*}
\int_{0}^{s}\left[\partial_{x x}^{2} H[t](\delta x(t), \delta y(t))+\partial_{x u}^{2} H[t](\delta x(t), \delta v(t))+\partial_{u x}^{2} H[t](\delta u(t), \delta y(t))\right] \mathrm{d} t \tag{2}
\end{equation*}
$$

Now, $\delta x=T \delta u$ where $T=j \circ T_{0}$ is the composition of the canonical injection $j: \mathrm{H}_{m}^{1}([0, s]) \hookrightarrow$ $\mathrm{L}_{m}^{2}([0, s])$ which is a compact operator [14], and of $T_{0} \in \mathscr{L}\left(\mathrm{~L}_{m}^{2}, \mathrm{H}_{m}^{1}\right)$ which maps $\delta u$ to $\delta x$. Then $T$ is compact on $\mathrm{L}_{m}^{2}$, and so is $R_{\mathrm{s}}$ as there is at least one left or right composition with $T$ in each term of (2). Moreover, $T$ can be represented as the integral Hilbert-Schmidt operator

$$
(T \delta u)(t)=\int_{0}^{t} \Phi(t-\sigma) \partial_{u} f[\sigma] \delta u(\sigma) \mathrm{d} \sigma
$$

where $\Phi$ is the fundamental solution of $\delta \dot{x}(t)=\partial_{x} f[t] \delta x(t)$. Then, denoting $|\cdot|$ the equivalent norm on $\mathrm{L}_{m}^{2}$, one has the estimate

$$
B_{\mathrm{s}}(\delta u, \delta u)=-|\delta u|^{2}+O(s)|\delta u|^{2}, \quad s \longrightarrow 0
$$

and the negative definiteness for small $s$ follows.
Clearly, if $s \leq t$, then $B_{t \mid K_{t}}<0$ implies $B_{\mathrm{s} \mid K_{\mathrm{s}}}<0$, hence the following definition. The first conjugate time along the extremal, $t_{1 c}$, is

$$
t_{1 c}=\sup \left\{s>0 \mid B_{\mathrm{s} \mid K_{\mathrm{s}}}<0\right\}
$$

Proposition 2.4 ([1]) Let $t_{1 c} \in\left(0, t_{\mathrm{f}}\right]$ for a regular extremal. Then $B_{t_{t_{c} \mid K_{t_{1 c}}}} \in \mathscr{L}\left(K_{t_{1 c} c}\right)$ has a non-trivial kernel.

Conjugate times are more generally defined as times $t_{\mathrm{c}}$ such that $B_{t_{\mathrm{c}} \mid K_{\mathrm{c}}}$ is degenerate. Points $\bar{x}\left(t_{c}\right)$ are then referred to as conjugate points. Under the Legendre condition, the equation $\partial_{u} H(x, u, p)=0$ can be solved in the neighbourhood of the extremal, yielding the smooth implicit function $u(x, p)$. Plugging $u(x, p)$ into $H$ defines the true Hamiltonian, $H(x, p)=H(x, u(x, p), p)$ (still denoted $H$, the number of arguments avoiding any ambiguity). Remarkably,

$$
\begin{aligned}
& \dot{\bar{x}}(t)=\partial_{p} H(\bar{x}(t), \bar{u}(t), \bar{p}(t))=\partial_{p} H(\bar{x}(t), \bar{p}(t)), \\
& \dot{\bar{p}}(t)=-\partial_{x} H(\bar{x}(t), \bar{u}(t), \bar{p}(t))=-\partial_{x} H(\bar{x}(t), \bar{p}(t)),
\end{aligned}
$$

which we write more compactly $\dot{\bar{z}}(t)=\vec{H}(\bar{z}(t))$, with $z=(x, p)$ and $\vec{H}=\left(\nabla_{p} H,-\nabla_{x} H\right)$ the symplectic gradient. A solution of the equation linearized along $\bar{z}$, the Jacobi equation,

$$
\delta \dot{z}(t)=\vec{H}^{\prime}(\bar{z}(t)) \delta z(t),
$$

is called a Jacobi field. Such a field $\delta z=(\delta x, \delta p)$ is said to be vertical at time $t$ whenever $\delta x(t)=0$. These notions allow us to characterize and compute conjugate times.

Proposition 2.5 An instant $s \in\left(0, t_{\mathrm{f}}\right]$ along a regular extremal is a conjugate time if and only if there exists a Jacobi field $\delta z=(\delta x, \delta p)$ vertical at 0 and $s$ such that $\delta x \not \equiv 0$ on $\left[0, t_{\mathrm{c}}\right]$.

Proof Let $\delta u \in \operatorname{Ker} B_{\mathrm{s} \mid K_{\mathrm{s}}}$, such that $\delta u \neq 0$. Then $B_{\mathrm{s}} \delta u$ must belong to $K_{\mathrm{s}}^{\perp}$. But $K_{\mathrm{s}}$ which is the closure in $\mathrm{L}_{m}^{2}$ of $\operatorname{Ker} F_{\mathrm{s}}^{\prime}(\bar{u})$ is also equal to $\operatorname{Ker} G_{\mathrm{s}}, G_{\mathrm{s}} \in \mathscr{L}\left(\mathrm{L}_{m}^{2}, \mathbf{R}^{n}\right)$ being the extension of $F_{\mathrm{s}}^{\prime}(\bar{u})$ to $\mathrm{L}_{m}^{2}$ (such an extension exists and remains continuous because $\bar{u}$ is bounded). Indeed, we have the following:

Lemma 2.6 Let $F$ be an everywhere dense subspace of a normed space, $E$, and let $G$ be finite-dimensional. Let $u \in \mathscr{L}(F, G)$, and let $v \in \mathscr{L}(E, G)$ be its continuous linear extension. Then $\operatorname{Ker} v=\overline{\operatorname{Ker} u}$.

Proof of Lemma One has $F=\operatorname{Ker} u \oplus H$ where $H \simeq \operatorname{Im} u$ and the direct sum is algebraic. As $G$ is finite-dimensional, the image of $u$ is closed so, by definition of $v, \operatorname{Im} u=\operatorname{Im} v$. Hence, $E=\operatorname{Ker} v \oplus H$ algebraically. Both $\operatorname{Ker} v$ and $H$ are closed, the latter being finite-dimensional, so the direct sum is also topological in $E$. Readily, $\operatorname{Ker} u \subset \operatorname{Ker} v$, so $\operatorname{Ker} u \times H \subset \operatorname{Ker} v \times H$. Since $E=\bar{F}$, $\operatorname{Ker} v \times H=\overline{\operatorname{Ker} u \times H}=\overline{\operatorname{Ker} u} \times \bar{H}=\overline{\operatorname{Ker} u} \times H$, whence the conclusion.

Thus, $K_{\mathrm{s}}^{\perp}=\left(\operatorname{Ker} G_{\mathrm{s}}\right)^{\perp}=\operatorname{Im} G_{\mathrm{s}}^{*}$, and there exists $\xi \in \mathbf{R}^{n}$ such that, for any $\delta v$ in $\mathrm{L}_{m}^{2}([0, s])$,

$$
B_{\mathrm{s}}(\delta u, \delta v)=\left(G_{\mathrm{s}}^{*} \xi \mid \delta v\right)_{\mathrm{L}_{m}^{2}}=\left(\xi \mid G_{\mathrm{s}} \delta v\right)_{\mathbf{R}^{n}}=\delta p(s) \delta y(s)
$$

with $\delta p$ being the covector-valued solution of

$$
\delta \dot{p}(t)=-\delta p(t) \partial_{x} f[t]-\bar{p}(t) \partial_{x x}^{2} f[t] \delta x(t)-\bar{p}(t) \partial_{u x}^{2} f[t] \delta u(t), \quad \delta p_{i}(s)=-\xi_{i}, \quad i=1, n,
$$

and $\delta x$ (resp. $\delta y$ ) associated to $\delta u$ (resp. $\delta v$ ) according to (1). Integrating by parts and compensating terms from both sides, one obtains

$$
\int_{0}^{s}\left[\partial_{u u}^{2} H[t](\delta u(t), \delta v(t))+\partial_{x u}^{2} H[t](\delta x(t), \delta v(t))+\partial_{p u}^{2} H[t](\delta p(t), \delta v(t))\right] \mathrm{d} t=0
$$

for arbitrary $\delta v$ so that on $[0, s]$

$$
\delta u(t)=-\left(\nabla_{u u}^{2} H[t]\right)^{-1}\left(\nabla_{x u}^{2} H[t] \delta x(t)+\nabla_{p u}^{2} H[t] \delta p^{\mathrm{T}}(t)\right) .
$$

Plugging this expression of $\delta u$ into the differential equations of $\delta x$ and $\delta p$, one verifies that $\delta z=(\delta x, \delta p)$ is a Jacobi fied. As $\delta u$ belongs to $K_{\mathrm{s}}=\operatorname{Ker} G_{\mathrm{s}}, \delta x(s)=G_{\mathrm{s}} \delta u=0$ and the field is vertical at 0 and $s$. Besides, if $\delta x \equiv 0$,

$$
0=B_{\mathrm{s}}(\delta u, \delta u)=\int_{0}^{s} \partial_{u u}^{2} H[t](\delta u(t), \delta u(t)) \mathrm{d} t \leq-\alpha\|\delta u\|_{\mathrm{L}_{m}^{2}}^{2}
$$

by the Legendre condition, so $\delta u$ would be zero, which is not. Conversely, let $\delta z=(\delta x, \delta p)$ be a Jacobi field vertical at 0 and $s, \delta x \not \equiv 0$. Setting

$$
\delta u(t)=-\left(\nabla_{u u}^{2} H[t]\right)^{-1}\left(\nabla_{x u}^{2} H[t] \delta x(t)+\nabla_{p u}^{2} H[t] \delta p^{\mathrm{T}}(t)\right),
$$

one has

$$
\begin{align*}
\delta \dot{x}= & \partial_{x}\left(\nabla_{p} H\right)(\bar{x}(t), \bar{p}(t)) \delta+\partial_{p}\left(\nabla_{p} H\right)(\bar{x}(t), \bar{p}(t)) \delta p(t) \\
& \partial_{x} f[t] \delta x(t)+\partial_{u} f[t] \delta u(t), \quad \delta x(0)=0 . \tag{3}
\end{align*}
$$

In particular, $\delta u \in K_{\mathrm{s}}$ as $\delta x(s)=0$. For $\delta v \in K_{\mathrm{s}}$, using the definition of $\delta u$,

$$
B_{\mathrm{s}}(\delta u, \delta v)=\int_{0}^{s}\left[\partial_{x x}^{2} H[t](\delta x(t), \delta v(t))+\partial_{u x}^{2} H[t](\delta u(t), \delta y(t))-\partial_{p u}^{2} H[t](\delta p(t), \delta v(t))\right] \mathrm{d} t .
$$

As

$$
\begin{aligned}
\delta \dot{p} & =\partial_{x}\left(-\nabla_{x} H\right)(\bar{x}(t), \bar{p}(t)) \delta x(t)+\partial_{p}\left(-\nabla_{x} H\right)(\bar{x}(t), \bar{p}(t)) \delta p(t) \\
& =-\delta p(t) \partial_{x} f[t]-\partial_{x x}^{2} f[t] \delta x(t)-\partial_{u u}^{2} f[t] \delta u(t),
\end{aligned}
$$

an integration by parts give

$$
\left.B_{\mathrm{s}}(\delta u, \delta v)=-\delta p(t) \delta y(t)\right]_{0}^{s}=0
$$

since $\delta v \in K_{\mathrm{s}}$ (so $\delta y(0)=\delta y(s)=0$ ). Therefore, $\delta u$ belongs to $\operatorname{Ker} B_{\mathrm{s} \mid K_{\mathrm{s}}}$. As $\delta u=0$ would imply $\delta x \equiv 0$ by virtue of (3), we conclude that $B_{\mathrm{s} \mid K_{\mathrm{s}}}$ has indeed a non-trivial kernel.

We finally formulate the second order necessary condition for regular extremals in the corank one analytic case. ${ }^{7}$

Theorem 2.7 [1,28] For a regular extremal associated with an analytic corank one optimal control, the absence of conjugate times on $\left(0, t_{\mathrm{f}}\right)$ is necessary for $\mathrm{L}^{\infty}$-local optimality.

Proof Suppose there exists a conjugate time $t_{\mathrm{c}} \in\left(0, t_{\mathrm{f}}\right)$. By definition, the kernel of $B_{t_{\mathrm{c}}} \mid K_{t_{\mathrm{c}}}$ is not trivial so one can find $0 \neq \delta u \in K_{t_{\mathrm{c}}}$ such that $B_{t_{\mathrm{c}}}(\delta u, \delta u)=0$. Let us define $\delta \tilde{u} \in K_{t_{\mathrm{f}}}$ as the extension of $\delta u$ by 0 on $\left[t_{\mathrm{c}}, t_{\mathrm{f}}\right]$, and check that it cannot belong to $\operatorname{Ker} B_{t_{\mathrm{f}} \mid K_{f_{f}}}$. If this were the case, then one could construct as in the proof of Proposition 2.5 a Jacobi field $\delta \tilde{z}=(\delta \tilde{x}, \delta \tilde{p})$ vertical at 0 and $t_{\mathrm{f}}$, such that $\delta \tilde{x} \not \equiv 0(\delta u \neq 0$, so $\delta \tilde{u} \neq 0)$. But as

$$
\delta \dot{\tilde{x}}(t)=\partial_{x} f[t] \delta \tilde{x}(t)+\partial_{u} f[t] \delta \tilde{u}(t), \quad \delta \tilde{x}\left(t_{\mathrm{f}}\right)=0
$$

$\delta \tilde{x}$ would identically vanish on $\left[t_{\mathrm{c}}, t_{\mathrm{f}}\right]$ (non-empty since $t_{\mathrm{c}}<t_{\mathrm{f}}$ ). Under the assumption that $\bar{u}$ is analytic, the Jacobi equation has analytic data and so analytic solutions. In particular, $\delta \tilde{x}$ would
identically vanish over $\left[0, t_{\mathrm{f}}\right]$, whence the contradiction. As $\delta \tilde{u} \notin \operatorname{Ker} B_{t_{\mathrm{f}} \mid K_{f_{\mathrm{f}}}}$, one can find $\delta \tilde{v} \in K_{t_{\mathrm{f}}}$ such that $B_{t_{\mathrm{f}}}(\delta \tilde{u}, \delta \tilde{v}) \neq 0$. Clearly, $B_{t_{\mathrm{f}}}(\delta \tilde{u}, \delta \tilde{u})=B_{t_{\mathrm{c}}}(\delta u, \delta u)=0$, so $B_{t_{\mathrm{f}}}$ takes opposite signs on the subspace generated by $\delta \tilde{u}$ and $\delta \tilde{v}$. It is then indefinite on $K_{t_{\mathrm{f}}}$, and so must be its restriction to Ker $F_{t_{\mathrm{c}}}^{\prime}(\bar{u})$. By virtue of Theorem 2.2, since $\bar{u}$ is a corank one critical point, $F_{t_{\mathrm{f}}}$ is locally open at $\bar{u}$ which prevents the point from being a local minimizer in $\mathrm{L}_{m}^{\infty}\left(\left[0, t_{\mathrm{f}}\right]\right)$.

It is clear from the proof that in the analytic situation, if the first conjugate point $t_{1 c}$ belongs to $\left(0, t_{\mathrm{f}}\right)$, then the following happens. Under the Legendre assumption, all operators $B_{\mathrm{s} \mid K_{\mathrm{s}}}$ are Fredholm and so diagonalizable on a Hilbert basis of eigenvectors. For $s<t_{1 c}$, all the eigenvalues are strictly negative. For $t_{1 c}$, finitely many of them vanish (the kernel of a Fredholm operator is finite-dimensional [14]). For $s>t_{1 c}$ at least one becomes positive, ensuring sign-indefiniteness. On the contrary, without analyticity, the kernel may remain non-trivial for $s>t_{1 c}$ with no positive eigenvalue appearing. The second-order intrinsic derivative may so remain negative semi-definite on a non-empty interval of conjugate times.

In contrast with finite-dimensional optimization, one cannot obtain a sufficient condition for optimality by a compactness argument. However, there is an even more satisfactory result asserting local optimality in a strong sense. Coming back to the initial control problem stated at the beginning of the section, we still assume that we have a regular extremal. Remembering that $\hat{x}=\left(x^{0}, x\right)$, the Pontryagin maximum principle in a strong form states that, if $\bar{u}$ is the bounded solution and $\bar{x}$ the associated Lipschitz trajectory, there exists a non-positive constant $p^{0}$ and a Lipschitz function $\bar{p}:\left[0, t_{\mathrm{f}}\right] \rightarrow\left(\mathbf{R}^{n}\right)^{*}$ such that almost everywhere on $\left[0, t_{\mathrm{f}}\right]$,

$$
\dot{x}(t)=\partial_{p} H(\bar{x}(t), \bar{u}(t), \bar{p}(t)), \quad \dot{p}(t)=-\partial_{x} H(\bar{x}(t), \bar{u}(t), \bar{p}(t)),
$$

and

$$
H(\bar{x}(t), \bar{u}(t), \bar{p}(t))=\max _{u \in U} H(\bar{x}(t), u, \bar{p}(t)),
$$

where ( $p^{0}$ appears as a parameter)

$$
H(x, u, p)=p^{0} f^{0}(x, u)+p f(x, u) .
$$

If the maximized Hamiltonian, $(x, p) \mapsto \max _{u \in U} H(x, u, p)$, is well defined and smooth in a neighbourhood of $\bar{z}$, then one necessarily has

$$
H(x, p)=H(x, u(x, p), p)=\max _{u \in U} H(x, u, p)
$$

on this neighbourhood under the Legendre condition (the implicit function $u(x, p)$ being locally the unique zero of $\partial_{u} H(x, \cdot, p)$, hence the only maximizer of $\left.H(x, \cdot, p)\right)$. These relations are homogenous in $\left(p^{0}, p\right)$ and there are two cases: The abnormal case, $p^{0}=0$, and the normal one, $p_{0}<0$. A control is said to be $\mathscr{C}^{0}$-locally optimal whenever there exists a neighbourhood of the associated trajectory in $\mathscr{C}^{0}\left(\left[0, t_{\mathrm{f}}\right], \mathbf{R}^{n}\right)$ such that any other admissible trajectory ${ }^{8}$ in this neighbourhood has a greater cost.

Theorem 2.8 For a normal regular extremal in the neighbourhood of which the maximized Hamiltonian is smooth, the absence of conjugate time on $\left(0, t_{f}\right]$ is sufficientfor $\mathscr{C}^{0}$-local optimality.

The proof is of completely different nature compared to the necessary condition. The argument is not spectral but relies on the geometric construction of the so-called field of extremals (see [1,8]). Summarizing, under appropriate assumptions, before first conjugate time local optimality holds on a large $\mathscr{C}^{0}$-neighbourhood of the trajectory, while past $t_{1 c}$ local optimality is lost, even in small $\mathrm{L}^{\infty}$-neighbourhoods.

## 3. Differential pathfollowing

Assume that we are given a family of optimal control problems parameterized by $\lambda \in[0,1]$ in the form of Section 2. For each $\lambda$, we minimize

$$
\int_{0}^{t_{\mathrm{f}}(\lambda)} f^{0}(x(t), u(t), \lambda) \mathrm{d} t \longrightarrow \min
$$

with fixed final time $t_{\mathrm{f}}(\lambda)>0$, subject to differential constraints on the fixed manifold $X$,

$$
\dot{x}(t)=f(x(t), u(t), \lambda), \quad u(t) \in U_{\lambda}, \quad t \in\left[0, t_{\mathrm{f}}(\lambda)\right],
$$

and boundary conditions

$$
x(0)=x_{0}(\lambda), \quad x\left(t_{\mathrm{f}}\right)=x_{\mathrm{f}}(\lambda) .
$$

As before, we assume that manifolds $U_{\lambda}$ are without boundary, and that all the data are smooth with respect to $(x, u, \lambda)$ (resp. $\lambda$ ). We make the following uniform assumption:

For all $\lambda \in[0,1]$, there exists a normal regular extremal $\left(x_{\lambda}, u_{\lambda}, p_{\lambda}\right)$ in the neighbourhood of which the maximized Hamiltonian is smooth, and along which Jacobi fields never become vertical for $t \in\left(0, t_{\mathrm{f}}(\lambda)\right]$.

See [13] for a refined analysis in the Riemannian setting. Let $\lambda_{0} \in[0,1]$. Under our assumption, the application

$$
\left(p_{0}, \lambda\right) \longmapsto x\left(t_{\mathrm{f}}(\lambda), x_{0}(\lambda), p_{0}, \lambda\right)
$$

mapping $\left(p_{0}, \lambda\right)$ to the value at $t_{\mathrm{f}}(\lambda)$ of the $x$-coordinate of the solution $z=(x, p)$ to

$$
\dot{z}(t)=\vec{H}(z(t), \lambda), \quad t \in\left[0, t_{\mathrm{f}}(\lambda)\right], \quad z(0)=\left(x_{0}(\lambda), p_{0}\right),
$$

is a smooth implicit function in a neighbourhood of $\left(p_{\lambda_{0}}(0), \lambda_{0}\right)$. Here, $H(x, p, \lambda)=$ $H(x, u(x, p, \lambda), p, \lambda)=\max _{u \in U} H(x, u, p, \lambda)$ where $u(x, p, \lambda)$ is implicitly defined thanks to the Legendre condition. Optimal control shooting is a coordinate-dependent computation and we must choose a fixed chart on $X$ whose domain contains the target points $x_{\mathrm{f}}(\lambda)$ in order to define the homotopy function [20]. In such coordinates,

$$
h\left(p_{0}, \lambda\right)=x\left(t_{\mathrm{f}}(\lambda), x_{0}(\lambda), p_{0}, \lambda\right)-x_{\mathrm{f}}(\lambda)
$$

is smooth on the previous neighbourhood, possibly shrinked so that $x_{\mathrm{f}}(\lambda)$ stays in the chart. Finding the solution $p_{\lambda_{0}}(0)$ of the $n$-dimensional shooting equation $h\left(\cdot, \lambda_{0}\right)=0$ provides us with an extremal along which no Jacobi field becomes vertical on $\left(0, t_{\mathrm{f}}\left(\lambda_{0}\right)\right]$. In particular, there is no conjugate time on $\left(0, t_{\mathrm{f}}\left(\lambda_{0}\right)\right.$ ] and we have a $\mathscr{C}^{0}$-locally optimal solution of optimal control problem with parameter $\lambda_{0}$. As target points $x_{\mathrm{f}}(\lambda)$ must remain in the chart not only for $\lambda$ close to $\lambda_{0}$ but for all $\lambda \in[0,1]$, we propose the following global framework.

Let $(x, \lambda) \mapsto \varphi(x, \lambda) \in \mathbf{R}^{n}$ be a parameterized chart defined on an open domain of the manifold (with boundary) $X \times[0,1]$. The graph $\left\{\left(x_{\mathrm{f}}(\lambda), \lambda\right), \lambda \in[0,1]\right\}$ of $x_{\mathrm{f}}$ has to be a subset of this domain. Consider similarly the cotangent space $T_{x_{0}(\lambda)}^{*}$ above each point of the graph of $x_{0}$ to define the fibre space

$$
\mathscr{F}=\bigcup_{\lambda \in[0,1]}\left\{x_{0}(\lambda)\right\} \times T_{x_{0}(\lambda)}^{*} \times\{\lambda\}
$$

which is an $(n+1)$-submanifold (with a boundary) of $T^{*} X \times[0,1]$. When the cotangent bundle is trivial, $T^{*} X \simeq X \times \mathbf{R}^{n}$, one simply has $\mathscr{F}=\mathbf{R}^{n} \times[0,1]$. The homotopy can then be globally
defined on some open subset $\mathscr{F}_{0}$ of $\mathscr{F}$ to $\mathbf{R}^{n}$ putting

$$
h(z, \lambda)=\varphi\left(x\left(t_{\mathrm{f}}(\lambda), x_{0}(\lambda), p_{0}, \lambda\right), \lambda\right)-\varphi\left(x_{\mathrm{f}}(\lambda), \lambda\right), \quad(z, \lambda)=\left(x_{0}(\lambda), p_{0}, \lambda\right) \in \mathscr{F}
$$

By restricting $\mathscr{F}_{0}$ if necessary, one can assume that it only contains regular points of $h$. As 0 is a regular value of the homotopy, each connected component of $h=0$ is a one-dimensional submanifold of $\mathscr{F}_{0}$, diffeomorphic either to $\mathbf{S}^{1}$ or to a real interval. A difficult issue is to provide sufficient conditions à la Smale [2] that ensure the existence of a component joining $\lambda=0$ to $\lambda=1$. Other issues include the following, as illustrated in the trivial case, $\mathscr{F}_{0}=\Omega \times[0,1]$ with $\Omega$ an open subset of $\mathbf{R}^{n}$. (i) Components diffeomorphic to real intervals must have their endpoints in the topological boundary of $\Omega \times[0,1]$. Such endpoints are critical points of the homotopy (the path could otherwise be prolonged), and bifurcations may occur [2]. (ii) Besides, for a fixed $\lambda$, one has to compare the costs associated to the zeros in each component of $h(\cdot, \lambda)=0$. This global aspect is responsible for possible loss of regularity - even discontinuity - of the value function (mapping $\lambda$ to the minimum value of the cost when it exists).

The connected component of the set of zeros starting at $\left(z_{\lambda=0}(0), 0\right)$ is a differentiable curve that we can parameterize by arc length ${ }^{9}, s$. In coordinates, $c(s)=\left(p_{\lambda(s)}(0), \lambda(s)\right)$ is a solution of the differential equation

$$
\begin{equation*}
\frac{\mathrm{d} c}{\mathrm{~d} s}(s)=\vec{T}(c(s)), \quad c(0)=\left(p_{\lambda=0}(0), 0\right) \tag{4}
\end{equation*}
$$

where $\vec{T}(c)$ is the unit tangent vector defined up to orientation by $\vec{T}(c) \in \operatorname{Ker} h^{\prime}(c)$ (c is not critical so the kernel is one-dimensional). As critical points are avoided, orientation is chosen so that the sign of

$$
\operatorname{det}\left[\operatorname{ker} h^{\prime}(c)^{\mathrm{T}} \vec{T}(c)\right]
$$

remains a constant. In contrast with established predictor-corrector methods (e.g. [31]), we follow the path of zeros by merely integrating the differential equation using a high-order numerical scheme without making any correction step.

## 4. Algorithmic aspects

The numerical integration of (4) uses a high order one step scheme with a variable stepsize. At each step, the tangent vector defining the right-hand side has to be computed. This essentially amounts to evaluating the differential of the homotopy (and then to reveal its kernel by standard linear algebra). In coordinates,

$$
\begin{aligned}
\partial_{p_{0}} h\left(p_{0}, \lambda\right) & =\partial_{p_{0}} x\left[p_{0}, \lambda\right] \\
\partial_{\lambda} h\left(p_{0}, \lambda\right) & =\partial_{t_{\mathrm{f}}} x\left[p_{0}, \lambda\right] t_{\mathrm{f}}^{\prime}(\lambda)+\partial_{x_{0}} x\left[p_{0}, \lambda\right] x_{0}^{\prime}(\lambda)+\partial_{\lambda} x\left[p_{0}, \lambda\right]-x_{\mathrm{f}}^{\prime}(\lambda),
\end{aligned}
$$

where $\left[p_{0}, \lambda\right]$ stands for $\left(t_{\mathrm{f}}(\lambda), x_{0}(\lambda), p_{0}, \lambda\right)$. The derivatives of $t_{\mathrm{f}}, x_{0}$ and $x_{\mathrm{f}}$ are straightforwardly computed by AD. As $x\left[p_{0}, \lambda\right]$ is the $x$-component of the solution evaluated at $t_{\mathrm{f}}$ of the system defined by the maximized Hamiltonian

$$
\partial_{t_{\mathrm{f}}} x\left[p_{0}, \lambda\right]=\nabla_{p} H\left(x\left[p_{0}, \lambda\right], p\left[p_{0}, \lambda\right]\right)
$$

where $p\left[p_{0}, \lambda\right]$ is the $p$-component of the same solution at $t_{\mathrm{f}}$. For the variational derivatives $\partial_{x_{0}} x$, $\partial_{p_{0}} x$ and $\partial_{\lambda} x$, the first option is to use plain finite differences. Now, it is numerically crucial in applications to use variable stepsize methods to compute adapted discretizations thanks to the local
error control (nested Runge-Kutta methods do so at very low cost). In this case, finite differences are known to behave poorly as the two grids dynamically computed to evaluate, say, $x\left[p_{0}, \lambda\right]$ and $x\left[p_{0}+\delta p_{0}, \lambda\right]$, may differ, generating an artificial non-differentiability. The workaround is to force the grid to remain the same when evaluating for $p_{0}+\delta p_{0}$. This is known as internal numerical derivative (IND, [7]). An alternative is to use AD on the integration code. Because of the variable stepsize, the code only defines a piecewise differentiable function, and AD actually computes the piecewise derivative, providing the same order of precision as IND for explicit one-step variable stepsize methods [23]. The last option is to explicitly assemble the variational system to compute Jacobi fields. As $\vec{H}^{\prime}$ is evaluated along the current solution, one has to integrate simultaneously $z$ and $\delta z$ systems ( $2 n+4 n^{2}$ dimensions to obtain the complete Jacobian with $\delta z$ a matrix of order $2 n$ ),

$$
\dot{z}(t)=\vec{H}(z(t), \lambda), \quad \delta \dot{z}(t)=\partial_{z} \vec{H}(z(t), \lambda), \quad z(0)=z_{0}, \quad \delta z(0)=I_{2 n}
$$

In the case of explicit one-step schemes with variable stepsize, AD on the integration code and VAR (integration of the augmented variational system) are identical provided the stepsize control in the latter case is made only on $z$-components (and not on ( $z, \delta z$ )). The same analysis holds for the variational derivative with respect to $\lambda$.

A byproduct of any of the three approaches, IND, AD or VAR, is the computation of Jacobi fields on $\left[0, t_{\mathrm{f}}(\lambda)\right]$ which allows us to verify numerically the assumption of Section 3. Let $\delta z^{i}$ be the Jacobi fields with initial conditions $\delta z^{i}(0)=\left(0, e_{i}\right), i=1, n$, used to compute $\partial_{p_{0}} x\left[p_{0}, \lambda\right]$ ( $\left\{e_{1}, \ldots, e_{n}\right\}$ being the canonical basis). The assumption that no Jacobi field along the extremal becomes vertical on $\left(0, t_{\mathrm{f}}(\lambda)\right]$ is equivalent to check that the rank of $\left\{\delta x^{i}(t), \ldots, \delta x^{n}(t)\right\}$ is equal to $n$ for $t \in\left(0, t_{\mathrm{f}}(\lambda)\right]$. In practice, a sign change in the determinant of the Jacobi fields can be monitored, with a drawback on the magnitude as the determinant is equal to the product of the singular values, all vanishing for $t=0$. A complementary test is thus to inspect the dynamics of the smallest singular value along the reference extremal.

The hampath compiler [17] implements these ideas. It extends cotcot [9,11] by adding the homotopy layer as described in Sections 3 and 4 and compiles a description via Fortran files of a regular family of optimal control problem into a collection of Matlab Mex-files. The entries are two files, hfun. f and bcfun.f defining, respectively, the smooth maximized Hamiltonian and the boundary conditions,

$$
H(t, x, p, \lambda): \mathbf{R} \times \mathbf{R}^{n} \times \mathbf{R}^{n} \times \mathbf{R} \longrightarrow \mathbf{R}, \quad b\left(z_{0}, t_{\mathrm{f}}, z_{\mathrm{f}}, \lambda\right): \mathbf{R}^{2 n} \times \mathbf{R} \times \mathbf{R}^{2 n} \times \mathbf{R} \longrightarrow \mathbf{R}^{2 n}
$$

The dynamics is not assumed to be autonomous and the final times may be left free, that is why $t$ and $t_{\mathrm{f}}$ appear in the list of arguments of $H$ and $b$, respectively. Boundary conditions are more general than what we have described and actually allow for initial and terminal constraints defined by proper submanifolds of the ambient manifold rather than single points (again parameterized by $\lambda$ ),

$$
x(0) \in X_{0, \lambda}, \quad x\left(t_{\mathrm{f}}\right) \in X_{f, \lambda} .
$$

Pontryagin maximum asserts that transversality conditions hold

$$
p(0) \perp T_{x(0)} X_{0, \lambda}, \quad p\left(t_{\mathrm{f}}\right) \perp T_{x\left(t_{\mathrm{f}}\right)} X_{f, \lambda},
$$

which, in coordinates, are translated into function $b$. In such a case, the absence of conjugate point along the reference extremal is still necessary but the condition is not sharp enough and one has to introduce focal points (see for instance [18] in the Riemannian case). The output of the compiler is a series of Mex-functions. Among these,


Figure 1. Overview of hampath.
expdhvfun exponentiates $\partial_{x} \vec{H}$, that is, integrates simultaneously the adjoint system in $z$ an its linearized to compute Jacobi fields. The ODE integrator is dopri5 [23] (explicit RungeKutta method of order 5 with a dense output).
ssolve seeks a zero of the homotopy shooting function for a single $\lambda$. Typically, it is used to compute the initial condition for pathfollowing. The Newton solver is hybrj [19] (modified Powell hybrid method). The Jacobian of the shooting function is computed by the VAR approach.
hampath follows the path of zero by merely integrating the differential equation (4).
As is clear from Figure 1 overview of the code organization, several first- and second-order derivatives have to be generated. This is done by AD using tapenade [24]. In addition to the derivatives listed at the beginning of the section, the symplectic gradient and its derivative (that is, the Hessian of $H$ up to some block permutation) are computed by AD, then are used to assemble the adjoint system and the Jacobi one as well.

## 5. Example 1: quantum control

We address the energy minimization problem for two-level dissipative quantum systems [10,12]. It consists in minimizing the $\mathrm{L}^{2}$-norm of the control over a fixed transfer time $t_{\mathrm{f}}$, while steering an initial state $q_{0}$ to a final state $q_{1}$. The state is $q=(x, y, z) \in \mathbf{R}^{3}$ and the dynamics is given by the control system

$$
\begin{aligned}
& \dot{x}=\Gamma x+u_{2} z, \\
& \dot{y}=-\Gamma y-u_{1} z, \\
& \dot{z}=\gamma_{-}-\gamma_{+}+u_{1} y-u_{2} x .
\end{aligned}
$$

This system is deduced from Kossakowski-Lindblad equations describing the dynamics of two-level dissipative quantum systems in the rotating wave approximation. Up to a proper renormalization, it corresponds to the Bloch equation in nuclear magnetic resonance (NMR), when the detuning term is zero. The dissipative parameters satisfy the constraint $2 \Gamma \geq \gamma_{+} \geq\left|\gamma_{-}\right|$, and the control is the complex function $u=u_{1}+\mathrm{i} u_{2}$ modelizing the action of an electromagnetic field. The cost corresponds to the energy transfer between the control field and the internal Hamiltonian and is an important physical issue. The Bloch ball $|q| \leq 1$, which is the physical state space of the system, is invariant for the dynamics. Such a control problem is motivated by two recent experimental research projects. The first one concerns the control of the rotation of a molecule in a gas phase using laser fields, while the second deals with the control of the spin dynamics by a magnetic field in NMR.

If we use spherical coordinates $x=\rho \sin \phi \cos \theta, y=\rho \sin \varphi \sin \theta, z=\rho \cos \theta$, then the state equation becomes

$$
\begin{aligned}
& \dot{\rho}=\gamma_{-} \cos \varphi-\rho\left(\delta \cos ^{2} \varphi+\Gamma\right) \\
& \dot{\theta}=-v_{1} \cot \varphi \\
& \dot{\varphi}=-\frac{\gamma_{-} \sin \varphi}{\rho}+\delta \sin \varphi \cos \varphi+v_{2}
\end{aligned}
$$

where $\delta=\gamma_{+}-\Gamma$ and the new control is $v=\mathrm{e}^{\mathrm{i} \theta} u=v_{1}+\mathrm{i} v_{2}$. Note, in particular, that the cost is invariant by this feedback as

$$
\int_{0}^{t_{\mathrm{f}}}\left(v_{1}^{2}+v_{2}^{2}\right) \mathrm{d} t=\int_{0}^{t_{\mathrm{f}}}\left(u_{1}^{2}+u_{2}^{2}\right) \mathrm{d} t .
$$



Figure 2. Energy minimization in quantum control, path of zeros. The initial adjoint state $p_{0} \in\left(\mathbf{R}^{3}\right)^{*}$ solution of the shooting function is computed when the homotopic parameter $\Gamma$ decreases from 3 to 2 .

The initial and final state are here $(\rho(0), \theta(0), \varphi(0))=(1,0, \pi / 4)$ and $\left(\rho\left(t_{\mathrm{f}}\right), \theta\left(t_{\mathrm{f}}\right), \varphi\left(t_{\mathrm{f}}\right)\right)=$ $0.3534,2.053,0.6004)$. The final time is set to $t_{\mathrm{f}}=0.5$. Parameters $\gamma_{+}$and $\gamma_{-}$are fixed, respectively, to 2 and 0.1 , and we are interested here in the evolution of the solution when the parameter $\Gamma$ is decreased from 3 to 2 . The corresponding path of zeros is portrayed in Figure 2. Optimal


Figure 3. Energy minimization in quantum control, controls. The two components of optimal controls for $\Gamma=3,2.75$, $2.5,2.25$ and 2 are portrayed, illustrating the change of strategy when the physical parameter $\gamma$ is decreased.


Figure 4. Energy minimization in quantum control, trajectories. Optimal trajectories in the Bloch ball are projected in the ( $x, z$ )-plane (upper subplot) and $(y, z)$-plane (lower subplot) for $\Gamma=3,2.75,2.5,2.25$ and 2.


Figure 5. Energy minimization in quantum control, second-order condition check. Along each extremal for $\Gamma=3$, $2.75,2.5,2.25$ and 2, three Jacobi fields are computed and the rank of $\left\{\delta x^{1}(t), \delta x^{2}(t), \delta x^{3}(t)\right\}$ is evaluated by singlular value decomposition (SVD). The evolution of the smallest singular value $\sigma_{3}$ is portrayed in each case (upper subplot). A careful check shows that it remains positive on $\left(0, t_{\mathrm{f}}\right]$ (even in the neighbourhood of $\Gamma=2.1$ ), so sufficient second-order conditions apply and settle $\mathscr{C}^{0}$-local optimality. The evolution of $\sigma_{3}\left(t_{\mathrm{f}}\right)$ along the path, directly connected to the rank condition of the homotopy, is also given (lower subplot).
controls and trajectories for intermediate $\Gamma$ are represented in Figures 3 and 4. Sufficient secondorder conditions are verified by a rank test on Jacobi fields along these extremals, see Figure 5, ensuring that we obtain $\mathscr{C}^{0}$-local optimal solutions of the problem in the whole range of physical parameters.

## 6. Example 2: Two-body control

Motivated by orbit transfer problems in space mechanics [3,27], we study the two-body controlled equation,

$$
\ddot{q}(t)=-\mu \frac{q(t)}{|q(t)|^{3}}+\frac{\varepsilon u(t)}{m}, \quad|u| \leq 1 .
$$

The position vector $q$ is in $\mathbf{R}^{3}$ and we restrict ourselves to non-collision elliptic orbits,

$$
q \times \dot{q} \neq 0, \quad \dot{q}^{2}<\frac{2 \mu}{|q|},
$$

which defines a six-dimensional state manifold here in the Cartesian coordinates. The control $u$ is prescribed to the unit Euclidean ball, $u_{1}^{2}+u_{2}^{2}+u_{3}^{2} \leq 1$, and $\varepsilon u / m$ where $m$ is the mass of the second-body models the acceleration at our disposal. Typically, $\varepsilon u$ is the thrust of a spacecraft in the central field of a planet (the first body) whose gravitation constant is $\mu$. For small $\varepsilon$, the trajectory is a perturbation of the integrable Keplerian motion. Dimension five coordinates
associated to first integrals that describe the geometry of the osculating ellipse, plus an angular position parameter, are well suited for numerical computations as all but the last one will be slowly varied during the motion. The semi-latus rectum $P$ and the eccentricity e prescribe the shape of the ellipse. The three Euler angles, $\Omega$ (precession angle or ascending node longitude), $i$ (nutation angle or inclination), $\theta$ (proper rotation or argument of perigee), prescribe the rotation of the orbit plane treated as a rigid body. Adding longitude, $l$, to define the position of the ellipse itself $(l-(\Omega+\theta)$ measures the polar angle with respect to semi-major axis in the orbit plane), we obtain a complete set of coordinates. Equivalently, we choose ( $P, e_{x}, e_{y}, h_{x}, h_{y}, l$ ) where the two vectors

$$
\left(e_{x}, e_{y}\right)=e(\cos (\Omega+\theta), \sin (\Omega+\theta)), \quad\left(h_{x}, h_{y}\right)=\tan \left(\frac{i}{2}\right)(\cos \Omega, \sin \Omega)
$$

are oriented by the semi-major axis (eccentricity vector) and the line of nodes, respectively. In these coordinates, the dynamics reads

$$
\dot{x}(t)=F_{0}(x(t))+\frac{\varepsilon}{m} \sum_{i=1}^{3} u_{i}(t) F_{i}(x(t))
$$

with

$$
\begin{aligned}
& F_{0}(x)=\sqrt{\frac{\mu}{P}} \frac{W^{2}}{P} \frac{\partial}{\partial l}, \\
& F_{1}(x)=\sqrt{\frac{P}{\mu}}\left(\sin l \frac{\partial}{\partial e_{x}}-\cos l \frac{\partial}{\partial e_{y}}\right), \\
& F_{2}(x)=\sqrt{\frac{P}{\mu}}\left(\frac{2 P}{W} \frac{\partial}{\partial P}+\left(\cos l+\frac{e_{x}+\cos l}{W}\right) \frac{\partial}{\partial e_{x}}+\left(\sin l+\frac{e_{y}+\sin l}{W}\right) \frac{\partial}{\partial e_{y}}\right), \\
& F_{3}(x)=\sqrt{\frac{P}{\mu}}\left(-\frac{Z e_{y}}{W} \frac{\partial}{\partial e_{x}}+\frac{Z e_{x}}{W} \frac{\partial}{\partial e_{y}}+\frac{C \cos l}{2 W} \frac{\partial}{\partial h_{x}}+\frac{C \sin l}{2 W} \frac{\partial}{\partial h_{y}}\right)
\end{aligned}
$$

and

$$
W=1+e_{x} \cos l+e_{y} \sin l, \quad Z=h_{x} \sin l-h_{y} \cos l, \quad C=1+h_{x}^{2}+h_{y}^{2}
$$

In contrast with Section 5, the cost functional is the $\mathrm{L}^{1}$-norm of the control,

$$
\int_{0}^{t_{f}}|u(t)| \mathrm{d} t \longrightarrow \min , \quad|u(t)|=\sqrt{u_{1}(t)^{2}+u_{2}(t)^{2}+u_{3}(t)^{2}},
$$

with free final time $t_{\mathrm{f}}$. Such a performance index models the fuel consumption (here with the approximation that the mass, $m$, remains constant) and is much more complicated than an $\mathrm{L}^{2}$-cost as is clear when applying the Pontryagin maximum principle.

The normal Hamiltonian to be maximized (the abnormal case is trivially eliminated here, so we set $p^{0}=-1$ ) is

$$
H(x, u, p)=-|u|+H_{0}(x, p)+\frac{\varepsilon}{m} \sum_{i=1}^{3} u_{i} H_{i}(x, p),
$$

where each $H_{i}(x, p)=p F_{i}(x)$ is the Hamiltonian lift of the corresponding vector field. Let us define the two switching functions

$$
\psi(x, p)=\left(H_{1}, H_{2}, H_{3}\right)(x, p), \quad \varphi(x, p)=-1+\frac{\varepsilon}{m} \psi(x, p) .
$$

On the open dense subset $\psi \neq 0$, the maximizer of $H(x, \cdot, p)$ on the unit Euclidean ball is

$$
u=\frac{\psi}{|\psi|} \quad \text { when } \varphi>0, \quad u=0 \quad \text { when } \varphi<0
$$

arbitrary if $\varphi$ vanishes. As a result, the control norm is bang-bang (equal to 0 or 1 ), and the problem is difficult to solve without a priori knowledge on the switching structure [26]. We therefore propose a standard interior penalization using a logarithmic barrier [4,5] to eliminate simultaneously the lack of regularity coming from the non-emptyness of the control set boundary $(|u|=1)$ and from the non-differentiability of the cost integrand at $u=0$. For $\alpha \in[0,1]$, consider the cost

$$
\int_{0}^{t_{\mathrm{f}}}[|u|-(1-\alpha) \ln |u|-(1-\alpha) \ln (1-|u|)] \mathrm{d} t
$$

for $u$ in the open pointed unit ball, $0<|u|<1$. Moreover, we combine this approach with a second perturbation putting

$$
\int_{0}^{t_{\mathrm{f}}}\{(1-\beta)+\beta[|u|-(1-\alpha) \ln |u|-(1-\alpha) \ln (1-|u|)]\} \mathrm{d} t .
$$

When $\beta$ is zero, the cost is $t_{\mathrm{f}}$ and we have the minimum time problem which is much simpler and well studied [16]. For $\beta=1$ and $\alpha=1$ the original problem is retrieved, while for $\beta \in[0,1]$ and $\alpha<1$, we are in the regular situation described in Sections 2 and 3. Another approach would consist in solving directly the target problem. Although second-order conditions that treat mixed control-state constraints are available [25], this would have two disadvantages in our view. First, one has to guess the number and location of junction points with the boundary of the constraint (whereas following the path turns numerically to capture the structure as illustrated in Figure 7). Moreover, these junction points set up new unknowns of the problem, making its solution even


Figure 6. $L^{1}$-minimization in two-body control, path of zeros. The initial adjoint state $p_{0} \in\left(\mathbf{R}^{6}\right)^{*}$ solution of the shooting function is computed when the homotopic parameter tends to 1 .


Figure 7. $L^{1}$-minimization in two-body control, norm of the controls. The norm of the three-dimensional control versus longitude (the final longitude is fixed whereas the final time is free) is displayed for $\lambda$ close to $0, \lambda=0.6$, and $\lambda$ close to 1 . For $\lambda=0$, the minimum time problem is solved and $|u|=1$ everywhere [16]. Conversely, for $\lambda$ close to 1 , the switching structure has been captured and almost-switches between 0 and 1 are observed on the norm.


Figure 8. $\mathrm{L}^{1}$-minimization in two-body control, optimal trajectory. The trajectory (in blue) around the Earth is displayed for $\lambda=0.999$, in three dimensions (upper subplot), $\left(q_{1}, q_{2}\right)$ and $\left(q_{2}, q_{3}\right)$-projections (lower subplots). The red arrows indicate the control in the three-dimensional view. The action of the control is clearly located around the apogees and the last two perigees.


Figure 9. $\mathrm{L}^{1}$-minimization in two-body control, second order condition check. Along each extremal for the previous values of $\lambda$, six Jacobi fields are computed and the rank of $\left\{\delta x^{1}(t), \ldots, \delta x^{6}(t)\right\}$ is evaluated by SVD. The evolution of the smallest singular value $\sigma_{6}$ over longitude is portrayed in each case (upper subplot). As it remains positive on $\left(0, t_{\mathrm{f}}(\lambda)\right]$, sufficient second-order conditions apply and settle $\mathscr{C}^{0}$-local optimality. The evolution of $\sigma_{6}\left(t_{\mathrm{f}}\right)$ along the path, directly connected to the rank condition of the homotopy, is also given (lower subplot).
$\operatorname{costlier}$ (for low thrusts, that is for small $\varepsilon$, there are hundreds of junctions). Rather than cascading the two homotopies, we use a single continuation $\lambda \mapsto(\alpha(\lambda), \beta(\lambda))$. The question of convergence when $\alpha \rightarrow 1$ is an issue though some hints can be found in the literature (see, e.g. [29,30]). See also [21,22] for results on this problem using another homotopy.

The results below solve a problem originally posed by the French Space Agency. A satellite of mass $m=1500 \mathrm{~kg}$ around the Earth $\left(\mu=398600.47 \mathrm{~km}^{3} \mathrm{~s}^{-2}\right)$ is to be transferred from an initial low, eccentric and inclined orbit towards the geostationary one using an $\varepsilon=10 \mathrm{~N}$ thrust. In our chart,

$$
\begin{aligned}
& P_{0}=11625 \mathrm{~km}, \quad e_{x 0}=0.75, \quad e_{y_{0}}=0, \quad h_{x 0}=0.612, \quad h_{y_{0}}=0, \quad l_{0}=\pi \mathrm{rad}, \\
& P_{\mathrm{f}}=42165 \mathrm{~km}, \quad e_{x \mathrm{f}}=0, \quad e_{y_{\mathrm{f}}}=0, \quad h_{x \mathrm{f}}=0, \quad h_{y_{\mathrm{f}}}=0, \quad l_{\mathrm{f}}=56 \mathrm{rad} .
\end{aligned}
$$

Numerical simulations are displayed for $\lambda$ between 0 and $1-1 e-3$. The corresponding path of zeros is portrayed in Figure 6. Optimal controls for intermediate $\lambda$ (close to 0, or close to 1) are represented Figure 7. The trajectory for $\lambda=0.999$ is at Figure 8. Sufficient second order conditions are verified by a rank test on Jacobi fields along these extremals, see Figure 9, ensuring that we obtain $\mathscr{C}^{0}$-local optimal solutions of the problem for $\lambda<1$.

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## Notes

1. Unless otherwise specified manifolds are supposed to be $\mathscr{C}^{\infty}$-smooth.
2. This does not exclude applications with bounded controls, though, as $U$ may be a compact submanifold. See also [15] ( $U=\mathbf{S}^{1}$ ) and [16] $\left(U=\mathbf{S}^{2}\right)$.
3. That is $\mathscr{C}^{\infty}$-smooth.
4. A mapping between topological spaces is locally open at a point if it sends neighbourhood of the point onto neighbourhoods of its image.
5. That is $\mathscr{C}^{\infty}$-smooth.
6. The application remains continuous though the topology is weakened because $\mathrm{L}^{2}([0, s])$ is a topological module over $\mathrm{L}^{\infty}([0, s])$.
7. In which case the manifolds $X, U$, and the data $\left(f^{0}, f\right)$ have to be assumed real analytic as well.
8. A trajectory with the fixed endpoints generated by a bounded control valued in $U$.
9. Under our assumption, the absence of conjugate point even implies that we can parameterize by $\lambda$, at least locally.

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[^0]:    *Corresponding author. Email: jean-baptiste.caillau@u-bourgogne.fr

