Geometric and numerical optimal control for microorganisms at low Reynolds number

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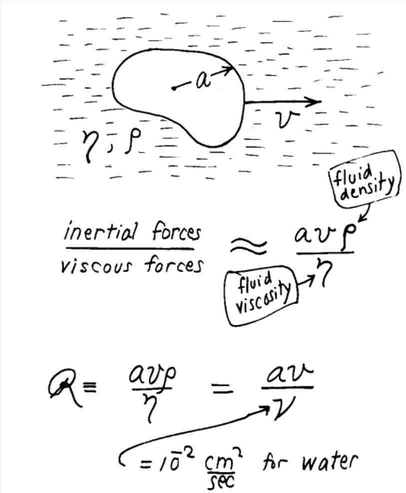
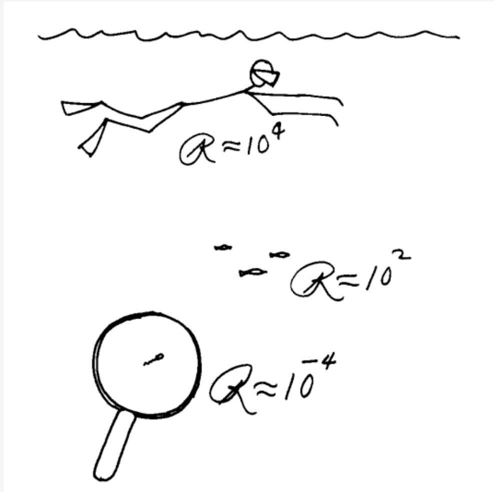
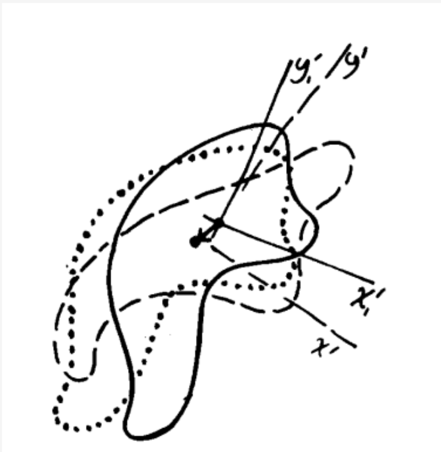
Life at low Reynolds number - Purcell, 1977

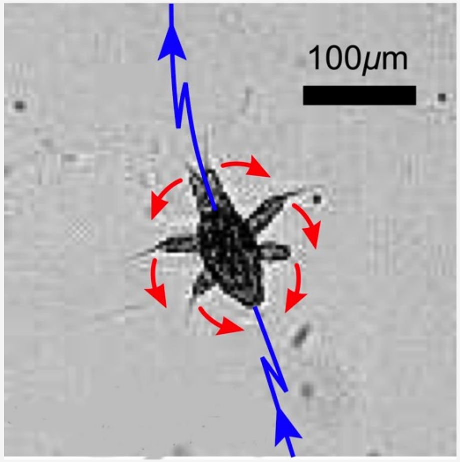




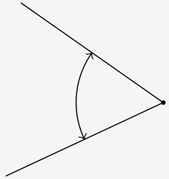
Reynolds number



Shape deformations



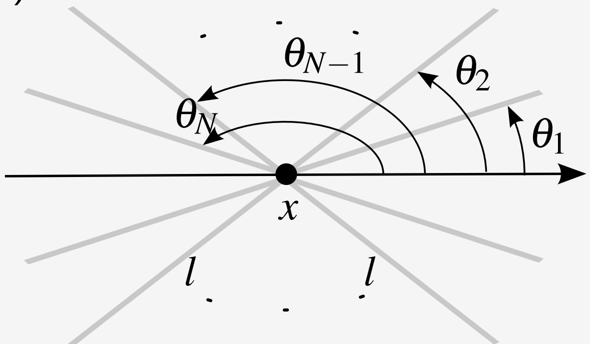
Zooplankton



Two-link swimmer: a scallop.

Theorem. *A scallop cannot swim.*

Symmetric N-link swimmer. Symmetric model of an abundant variety of zooplankton (Takagi 2014).



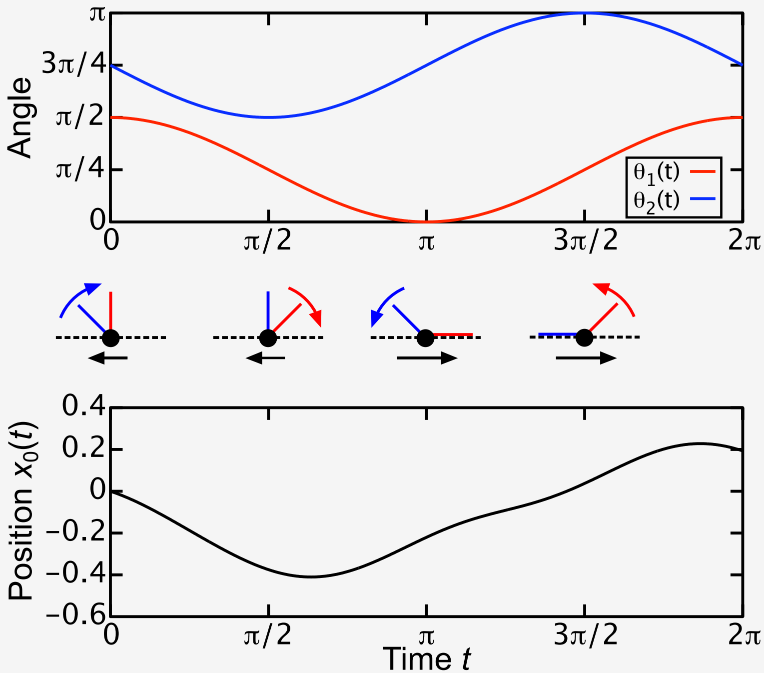
Controlled dynamics.

$$\dot{x} = \frac{\sum_{i=1}^{N} l\,\dot{\theta}_i \sin(\theta_i)}{n + \sum_{i=1}^{N} \sin^2(\theta_i)}, \quad \dot{\theta}_i = u_i,\ i = 1, \dots N \quad \text{(constraint: } 0 \leq \theta_1 \leq \dots \theta_N \leq \pi).$$

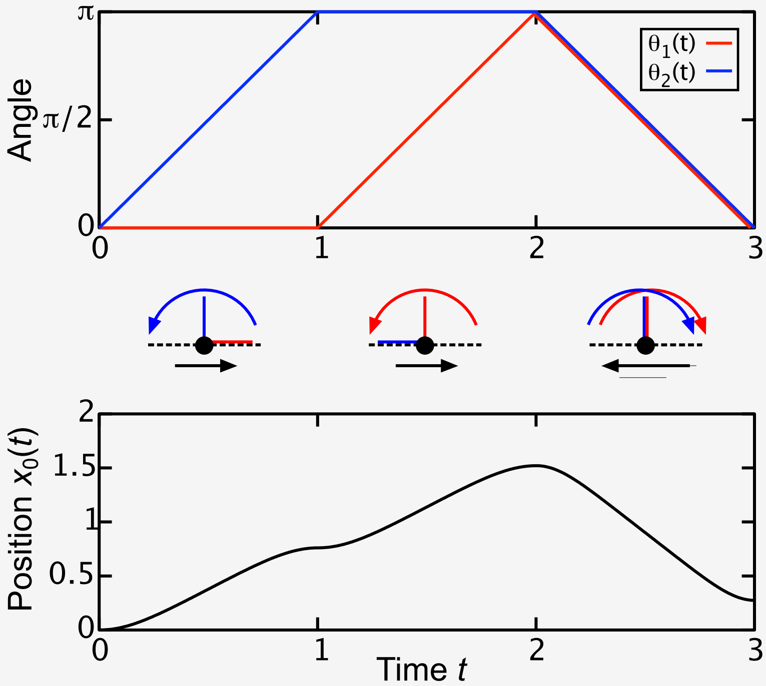
Minimize the Mechanical energy. $\dot{q}M(q)\dot{q}^t$ where $q = (x, \theta_1, \dots, \theta_N)$ and M is a positive-definite matrix $\Longrightarrow$ quadratic form in $(u_1, \dots, u_N)$.

Definition. *A stroke is a* **periodic motion** *of the shape variables* (θ_1, θ_2) *associated with a periodic control producing a* **net displacement** *of the position variables after one period* T *(we can fixed* $T = 2\pi$*).*

First case: Trigonometric controls.



Second case: Piecewise linear periodic control.



- The driftless control system is

$$\dot{q}(t) = \sum_{i=1}^{2} u_i(t) F_i(q(t))$$

where $q = (x, \theta_1, \theta_2)$, $F_i = \frac{\sin(\theta_i)}{\Delta} \frac{\partial}{\partial x} + \frac{\partial}{\partial \theta_i}$ and $\Delta = 2 + \sin^2(\theta_1) + \sin^2(\theta_2)$.

$$\dot{z} = u_1 \overrightarrow{H_1}(z) + u_2 \overrightarrow{H_2}(z), \quad z = (q, p)$$

where $\overrightarrow{H_i}$ are the Hamiltonian vector fields of the Hamiltonian lifts $H_i(z) = \langle p, F_i(q) \rangle$, $i = 1, 2$.

- **Pontryagin Maximum Principle:**

$\exists\, p(.) \in W^{1,1}([0,T]; \mathbb{R}^2)$ and a constant $p^0 \leq 0$ such that for a.e. $t \in [0,T]$,

  - $(p(.), p^0) \neq (0,0)$
  - $\frac{\partial H}{\partial u} = 0$ where $H(z, p^0, u) = u_1 H_1(z) + u_2 H_2(z) + p^0 (a(q) u_1^2 + 2b(q) u_1 u_2 + c(q) u_2^2)$

- Two types of extremals:

$p_0 = -1/2$: **normal extremals** given by the true Hamiltonian

$$H_n = \frac{1}{2}(a(q) u_1^{*2} + 2b(q) u_1^* u_2^* + c(q) u_2^{*2}).$$

$p_0 = 0$: **abnormal extremals**.

Abnormal curves. We have $H_1(z) = H_2(z) = \{H_1, H_2\}(z) = 0$ and the controls are given by

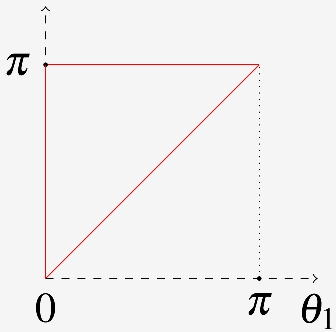
$$u_1^* \{\{H_1, H_2\}, H_1\}(z) + u_2^* \{\{H_1, H_2\}, H_2\}(z) = 0.$$

Computations for the copepod swimmer.

Lemma. *The surface* $\Sigma : \{q;\ \det(F_1(q), F_2(q), [F_1, F_2](q)) = 0\}$ *contains abnormal curves and is given by*

- $\theta_i = 0$ *or* π*, for* $i = 1, 2$*,*
- $\theta_1 = \theta_2$*.*

It is formed by the **boundary of the physical domain***:* $\theta_i \in [0, \pi]$, $i = 1, 2, \theta_1 \leq \theta_2$*, with respective controls* $u_1 = 0$*,* $u_2 = 0$ *or* $u_1 = u_2$*.*



: abnormal curve
in the (θ_1, θ_2)-plane

Remark. *A recent contribution proves that a trajectory with a corner of this type cannot be optimal.*

$H_3 = \langle p, F_3(q)\rangle$, with $F_3 = [F_1, F_2]$ and the set $\{q, H_1, H_2, H_3\}$ are coordinates. (the problem is isoperimetric since p_1 is a first integral: $\dot{p}_1 = 0$).

Equations in the Poincaré coordinates.

$$\dot{H}_1 = dH_1(\overrightarrow{H}_n) = \{H_1, H_2\} H_2 = H_2 H_3,$$
$$\dot{H}_2 = dH_2(\overrightarrow{H}_n) = \{H_2, H_1\} H_1 = -H_1 H_3,$$
$$\dot{H}_3 = dH_3(\overrightarrow{H}_n) = \{H_3, H_1\} H_1 + \{H_3, H_2\} H_2$$

with $\{H_3, H_1\}(z) = \langle p, [[F_1, F_2], F_1](q)\rangle$, $\quad \{H_3, H_2\}(z) = \langle p, [[F_1, F_2], F_2](q)\rangle$.
At a *contact point* $\{F_1, F_2, F_3\}$ forms a frame, therefore

$$[[F_1, F_2], F_1](q) = \sum_{i=1}^{3} \lambda_i(q) F_i(q), \quad [[F_1, F_2], F_2](q) = \sum_{i=1}^{3} \lambda_i'(q) F_i(q),$$

and computing one gets,

$$\lambda_1 = \lambda_2 = 0, \frac{\partial f}{\partial \theta_1} = \lambda_3 f \text{ and } \lambda_1' = \lambda_2' = 0, \frac{\partial f}{\partial \theta_2} = \lambda_3' f.$$

We conclude that

$$\dot{H}_1 = H_2 H_3, \quad \dot{H}_2 = -H_1 H_3,$$
$$\dot{H}_3 = H_3 \left(\lambda_3 H_1 + \lambda_3' H_2\right).$$

Integration. Time reparameterization: $ds = H_3 dt$

$$\frac{dH_1}{ds} = H_2, \qquad \frac{dH_2}{ds} = -H_1, \qquad \frac{dH_3}{ds} = \lambda_3 H_1 + \lambda_3' H_2.$$

Hence $H_1'' + H_1 = 0$ when differentiating with respect to the new time s (harmonic oscillator).
Furthermore with the approximation λ_3, λ_3' constant,

$$\frac{dH_3}{ds} = A\cos(s+\rho).$$

We obtain, up to reparameterization, **trigonometric functions for the controls.**

Applying the PMP, we solve numerically boundary value problem:

$$\begin{cases} \dot{q} = \frac{\partial H_n}{\partial p}, \qquad \dot{p} = -\frac{\partial H_n}{\partial q}, \\ x(0) = 0, \quad x(2\pi) = x_f, \\ \theta_i(0) = \theta_i(2\pi),\ i = 1,2 \quad p_j(0) = p_j(2\pi),\ j = 2,3 \end{cases}$$

where H_n is the true Hamiltonian in the normal case.
Two software used:

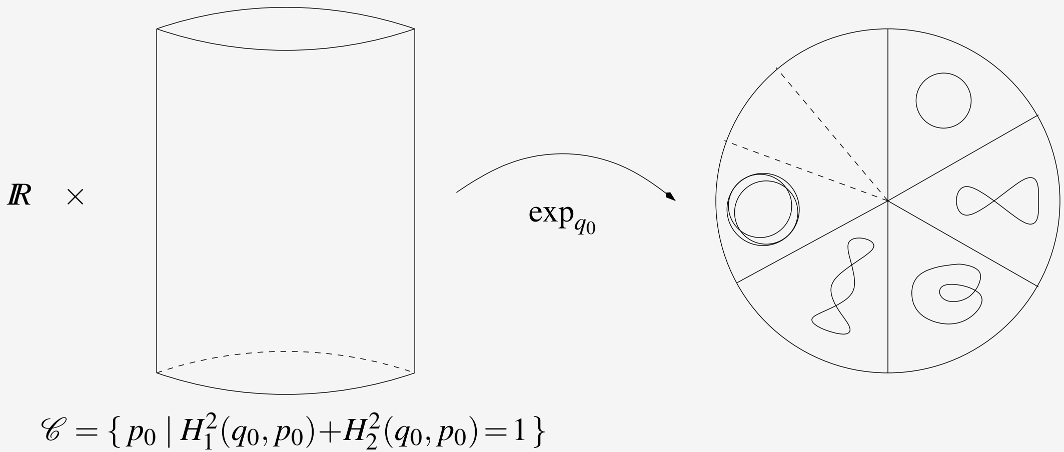
- `Bocop` (*direct method*: discretization of the state and control spaces → NLP problem) gives an initialisation for the shooting algorithm of the `HamPath` software.
- `HamPath` (*indirect method*: shooting algorithm, homotopic methods) solve the boundary value problem and compute **necessary second order optimality conditions**.

First conjugate time t_c: the exponential map

$$\exp_{q_0} : \mathbb{R} \times \mathscr{C} \to M, \quad (t, p_0) \mapsto q(t, q_0, p_0)$$

is not immersive at (t_c, p_0).

Theorem. *Let $q : [0, T] \longrightarrow \mathbb{R}^n$ be a strict normal stroke. If $q(.)$ has at least one conjugate point on $]0, T[$, then q* **is not a local minimizer** *in the L^∞-topology for controls and considering the problem with fixed extremities.*



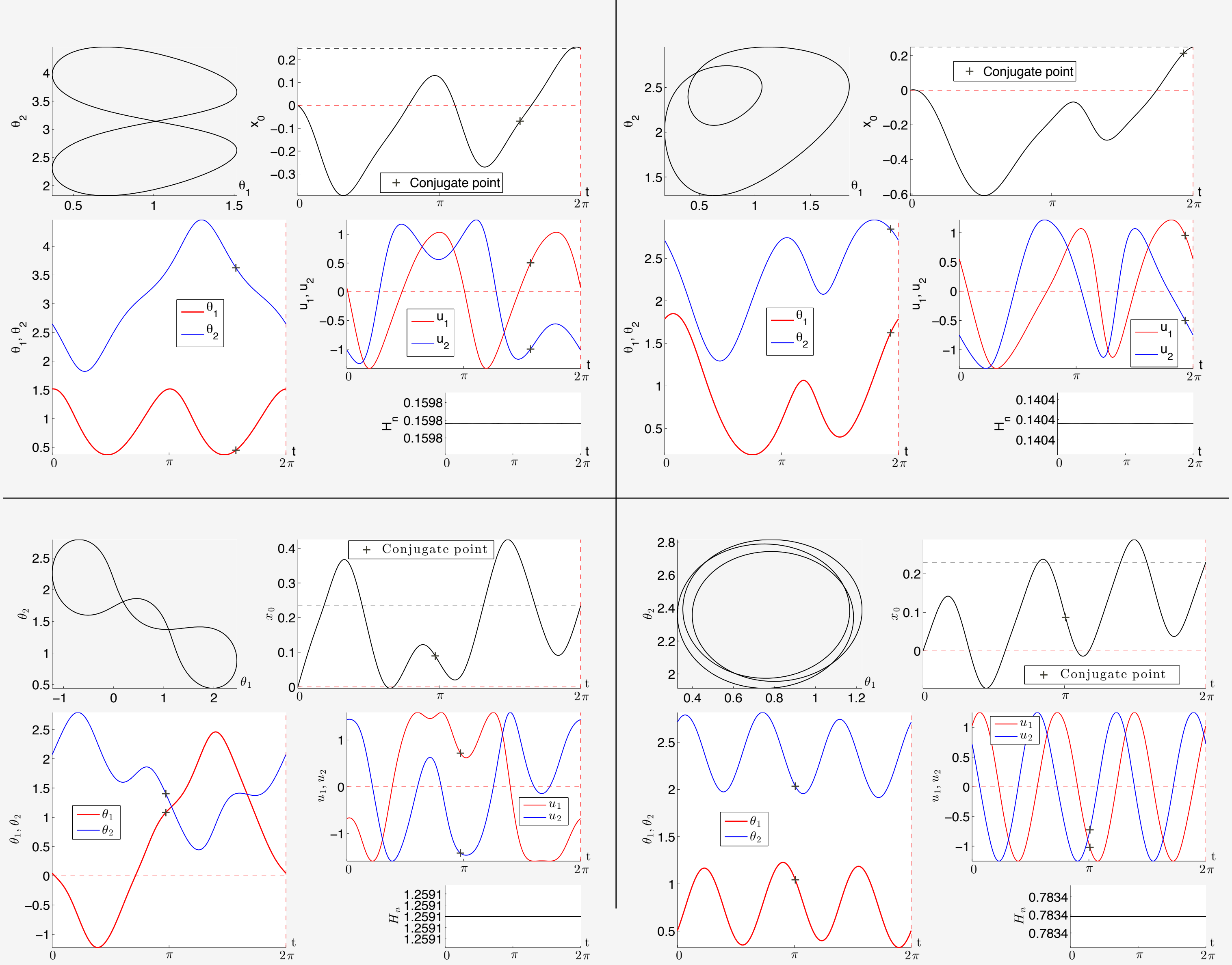
Let $z(.) = (q(.), p(.))$ be a normal extremal of the Hamiltonian system defined by $\overrightarrow{H_n}$. The variational equation is

$$\dot{\delta z}(t) = \frac{\partial \overrightarrow{H}_n}{\partial z}(q(t), p(t))\delta z(t).$$

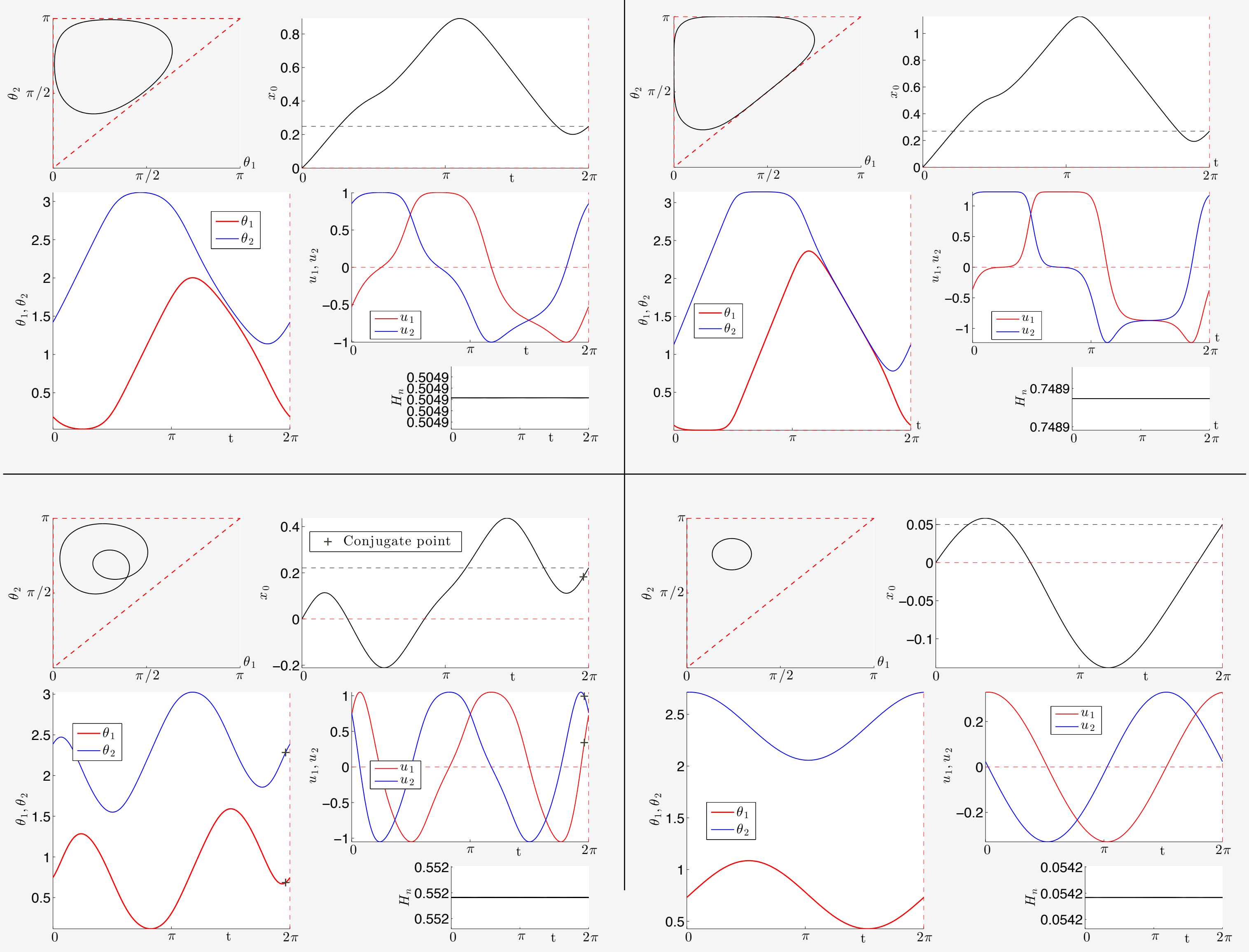
A time $t_c \in]0, T]$ is a conjugate time if there exists a Jacobi field $\delta z = (\delta q, \delta p)$, that is a non-zero solution of the variational equation such that $\delta q(0) = \delta q(t_c) = 0$.

We denote $\delta z_i = (\delta q_i, \delta p_i),\ i = 1...3$, three linearly independent Jacobi fields with initial condition $\delta q(0) = 0$. At time t_c we have the following rank condition

$$\textbf{rank}\{\boldsymbol{\delta q_1(t_c), \delta q_2(t_c), \delta q_3(t_c)}\} < \mathbf{3}.$$



θ2
θ1
x0
t
Conjugate point
θ1, θ2
θ1
θ2
u1, u2
u1
u2
Hn
0.1598
0.1404
1.2591
0.7834
0
π
2π


+ Conjugate point
θ_1
θ_2
u_1
u_2
x_0
H_n
θ_1, θ_2
u_1, u_2
t
0.5049
0.7489
0.552
0.0542

Augmented state: $\overline{q} = (q, q^0)$ where $q^0(.)$ is the mechanical cost.
Among extremals which minimize the mechanical energy, we want to find the one which minimizes a function $g(\overline{q}(0), \overline{q}(T))$.

(OCP)

$$\min\ g(\overline{q}(0), \overline{q}(T))$$

subject to bounded measurable functions $u : [0,T] \to \mathbb{R}^m$ and arcs $\overline{q} \in W^{1,1}([0,T];\mathbb{R}^n)$ satisfying

$$\dot{\overline{q}}(t) = f(\overline{q}(t), u(t)) \quad \text{a.e. } t \in [0,T],$$

$$u(t) \in U \subset \mathbb{R}^m \quad \text{a.e. } t \in [0,T],$$

$$(\overline{q}(0), \overline{q}(T)) \in C \subset \mathbb{R}^{2n}$$ (C is smooth and closed).

Transversality conditions

$$(\overline{p}(0), -\overline{p}(T)) \in \lambda \nabla_{\overline{q}(0),\overline{q}(T)} g(\overline{q}(0), \overline{q}(T)) + N_C(\overline{q}(0), \overline{q}(T))$$

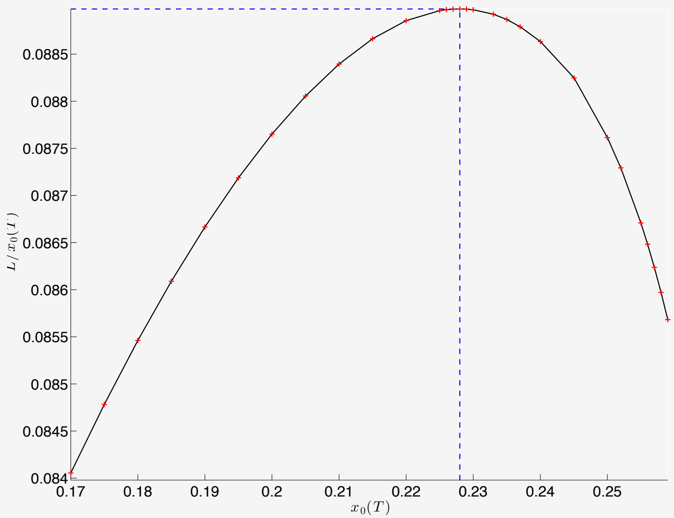
where $N_C(x)$ is (reduced) to the set of outward normals at x.

Comparisons of strokes

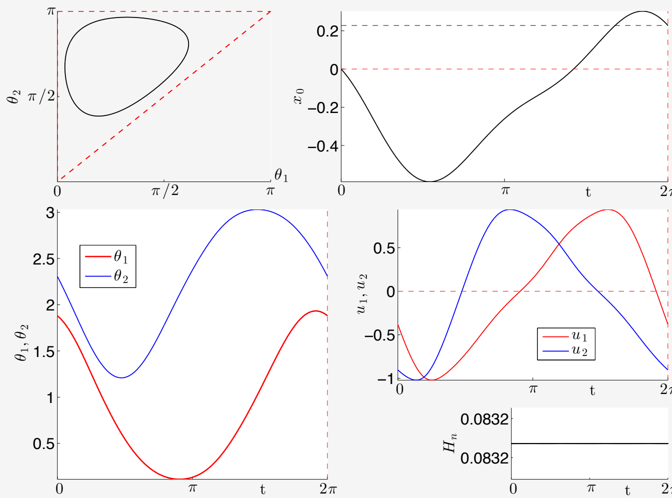
The **geometric efficiency** of a stroke γ is defined by the ratio $\boldsymbol{x/L(\gamma)}$,

- $L(\gamma)$ is the length of the stroke γ (*independent of the time parameterization*),
- x the corresponding displacement.

"Simple loops" are the only strokes without conjugate points.

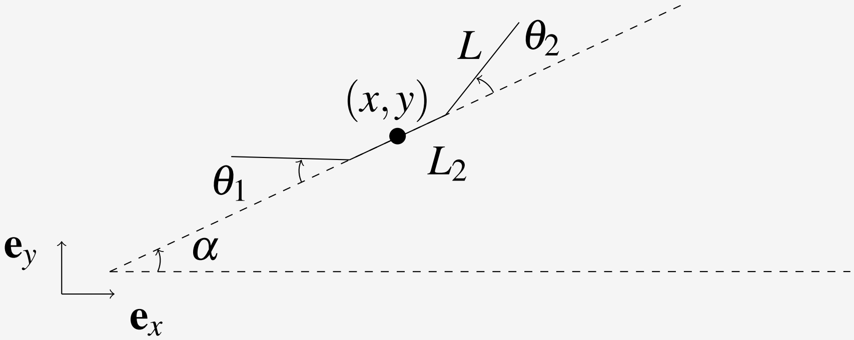


Curves of efficiencies obtained by continuation on $x(T)$.



Stroke corresponding to the maximum of efficiency.

Three-link swimmer: the Purcell swimmer.



Dynamic.

$$\dot{q} = D(\alpha)G(\theta)\dot{\theta}, \qquad D(\alpha) = \begin{pmatrix} \cos(\alpha) & -\sin(\alpha) & 0 \\ \sin(\alpha) & \cos(\alpha) & 0 \\ 0 & 0 & 1 \end{pmatrix},$$

$$\dot{\theta} = H(\theta)\tau, \qquad \tau \text{ is the torque}, \quad \theta = (\theta_1, \theta_2), \quad q = (x, y, \alpha).$$

The control is given by $u := \dot{\theta}$. G and H have complicated expressions, this is a complex problem even locally.

Mechanical energy to minimize. Work of the drag forces $E(u) = \int_0^T (uH^{-1}u)\mathrm{d}t$.

Optimal control problem.

$$\dot{X} = u_1 F_1(X) + u_2 F_2(X), \quad X = (\theta_1, \theta_2, x, y, \alpha).$$

Sub-Riemannian geometry. (M, D, g) where M is an $n-$dimensional manifold, D a distribution of constant rank $m \leq n$ and g is a Riemannian metric on D.

$$D_1 = \text{span}\{F_1, F_2\},\ D_2 = D_1 \cup \text{span}\{[F_1, F_2]\},$$
$$D_3 = D_2 \cup \text{span}\{[[F_1, F_2], F_1], [[F_1, F_2], F_2]\}$$

At a point X_0, $D_1(X_0)$ is a $(2,3,5)-$distribution.

- compute the **nilpotent approximation** $(\hat{F}_1, \hat{F}_2)$,
- integrate analytically the nilpotent extremal system,
- compute numerically strokes from the nilpotent extremal system,
- continuation techniques to obtain strokes of the real system.

Aim: Compute a tangent structure which approximate the tangent space of a SR manifold (which has also the SR structure).

Given a distribution $D : M \to TM$. Near x_0, $D(x_0) = \mathrm{span}\{F_1(x_0), \ldots, F_m(x_0)\}$.

- compute orders and weights of functions and vector fields $\to$ compute privileged coordinates.
- the approximate vector fields generate a **nilpotent Lie algebra** with dilations.

Theorem. *The nilpotent approximation (of order* -1*) at zero is*

$$\hat{F}_1 = \frac{\partial}{\partial x_1} + O(|x|^3), \quad \hat{F}_2 = \frac{\partial}{\partial x_2} + x_1 \frac{\partial}{\partial x_3} + \frac{\partial}{\partial x_4} + x_1^2 \frac{\partial}{\partial x_5} + O(|x|^3).$$

Proof. Actions such that $\theta_1 = x_1$ and $\theta_2 = x_2$ are invariant:

- action of a diffeomorphism φ on the vector fields F, G:

$$\varphi \cdot (F, G) = (\varphi_*(F), \varphi_*(G))$$

- action of a formal series α on the vector fields F, G:

$$\alpha \cdot (F, G) = (F\cos(\alpha) + G\sin(\alpha), -F\sin(\alpha) + G\cos(\alpha)).$$

□

We have an explicit relation between the **physical coordinates** $(\theta_1, \theta_2, x, y, \alpha)$ and the **coordinates of the nilpotent approximation** $(x_i)_{i=1,\dots,5}$.

SR problem. Cartan flat case:

$$\dot{x} = \sum_{i=1}^{2} u_i \hat{F}_i, \quad \min_u \int_0^T (u_1^2 + u_2^2)\,dt.$$

Pontryagin maximum principle. If $x(.)$ is optimal then $(x(.), p(.))$ is solution of the system given by the Hamiltonian:

$$H(x,p) = \frac{1}{2}(H_1(x,p)^2 + H_2(x,p)^2).$$

Hamiltonian lifts.

$$H_1 = \langle p, \hat{F}_1(x) \rangle = p_1, \qquad H_2 = \langle p, \hat{F}_2(x) \rangle = p_2 + p_3 x_1 + p_4 x_3 + p_5 x_1^2,$$
$$H_3 = \langle p, [\hat{F}_1, \hat{F}_2](x) \rangle = -p_3 - 2x_1 p_5, \quad H_4 = \langle p, [[\hat{F}_1, \hat{F}_2], \hat{F}_1](x) \rangle = -2p_5,$$
$$H_5 = \langle p, [[\hat{F}_1, \hat{F}_2], \hat{F}_2](x) \rangle = p_4.$$

We consider Poincaré coordinates $(H_1, H_2, H_3, H_4, H_5)$

$$\dot{H}_1 = dH_1(\overrightarrow{H}) = \{H_1, H_2\}H_2 = \langle p, [\hat{F}_1, \hat{F}_2](x)\rangle H_2 = H_2 H_3,$$

$$\begin{aligned} \dot{H}_2 &= -H_3 H_1, & \dot{H}_3 &= H_1 H_4 + H_2 H_5, \\ \dot{H}_4 &= 0 \quad \text{hence} \quad H_4 = c_4, & \dot{H}_5 &= 0 \quad \text{hence} \quad H_5 = c_5. \end{aligned}$$

Fixing the level energy $H_1^2 + H_2^2 = 1$, we set $H_1 = \cos(\theta)$ and $H_2 = \sin(\theta)$.

$$\dot{H}_1 = -\sin(\theta)\dot{\theta} = H_2 H_3 = \sin(\theta) H_3.$$

Hence $\dot{\theta} = -H_3$ and

$$\ddot{\theta} = -(H_1 c_4 + H_2 c_5) = -c_4 \cos(\theta) - c_5 \sin(\theta) = -\omega^2 \sin(\theta + \phi)$$

where ω and ϕ are constants.
By identification, we get $\omega^2 \sin(\phi) = c_4$ and $\omega^2 \cos(\phi) = c_5$.
Let $\psi = \theta + \phi$, we get

$$\frac{1}{2}\dot{\psi}^2 - \omega^2 \cos(\psi) = B,$$

where B is a constant.

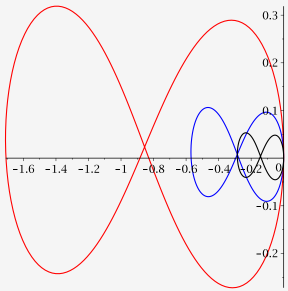
Oscillating case. We set $u = \omega t + \varphi_0$, k is the modulus of elliptic functions

$$k(\hat{p}(0)) = \frac{1}{2}\sqrt{\frac{2\sqrt{\hat{p}_4(0)^2 + 4\,\hat{p}_5(0)^2} + \hat{p}_3(0)^2 - 2\,\hat{p}_1(0)\,\hat{p}_4(0) - 4\,\hat{p}_5(0)\,\hat{p}_2(0)}{\sqrt{\hat{p}_4(0)^2 + 4\,\hat{p}_5(0)^2}}}$$

Compute $\hat{p}(0)$ such that the analytic solutions

$$x_1(u) = \frac{1}{\omega}\left[x_1(\varphi_0) - 2k\sin(\phi)\,\mathrm{cn}(u,k) + (-u + 2E(u,k))\cos(\phi)\right],$$
$$x_2(u) = \frac{1}{\omega}\left[x_2(\varphi_0) - 2k\cos(\phi)\,\mathrm{cn}(u,k) + (u - 2E(u,k))\sin(\phi)\right],$$
$$x_3(u)\ldots, x_4(u)\ldots, x_5(u)\ldots$$

give periodic strokes (of period $T = 4K(k)/(\hat{p}_4(0)^2 + 4\,\hat{p}_5(0)^2)^{1/4}$).



Family of eight shape strokes in the (x_1, x_2)-plane.

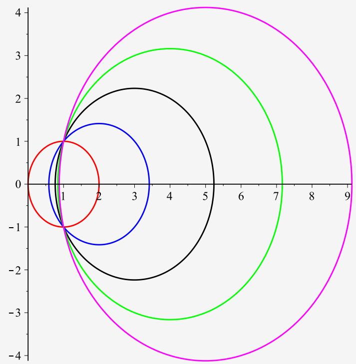
Rotating case. The modulus can be expressed as

$$k(\hat{p}(0)) = 2\sqrt{\frac{\sqrt{\hat{p}_4(0)^2+4\,\hat{p}_5(0)^2}}{2\sqrt{\hat{p}_4(0)^2+4\,\hat{p}_5(0)^2}+\hat{p}_3(0)^2-2\,\hat{p}_1(0)\,\hat{p}_4(0)-4\,\hat{p}_5(0)\,\hat{p}_2(0)}}$$

Compute $\hat{p}(0)$ such that the analytic solutions

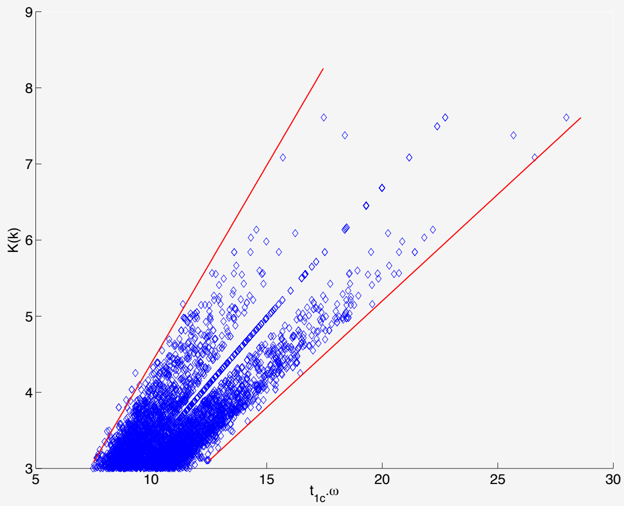
$$x_1(u) = \left(-2\cos(\phi)\,u + 2\cos(\phi)\,\mathrm{E}(u/k,k)\,k - 2\sin(\phi)\,\mathrm{dn}(u/k,k)\,k + \cos(\phi)\,uk^2 + x_1(\varphi_0)\,k^2\right)\omega^{-1}k^{-2},$$
$$x_2(u) = \left(2\sin(\phi)\,u - 2\sin(\phi)\,\mathrm{E}(u/k,k)\,k - 2\cos(\phi)\,\mathrm{dn}(u/k,k)\,k - \sin(\phi)\,uk^2 + x_2(\varphi_0)\,k^2\right)\omega^{-1}k^{-2},$$
$$x_3(u)\ldots, x_4(u)\ldots, x_5(u)\ldots$$

give periodic strokes (of period $T = 2\pi/(\hat{p}_4(0)^2 + 4\,\hat{p}_5(0)^2)^{1/4}$).

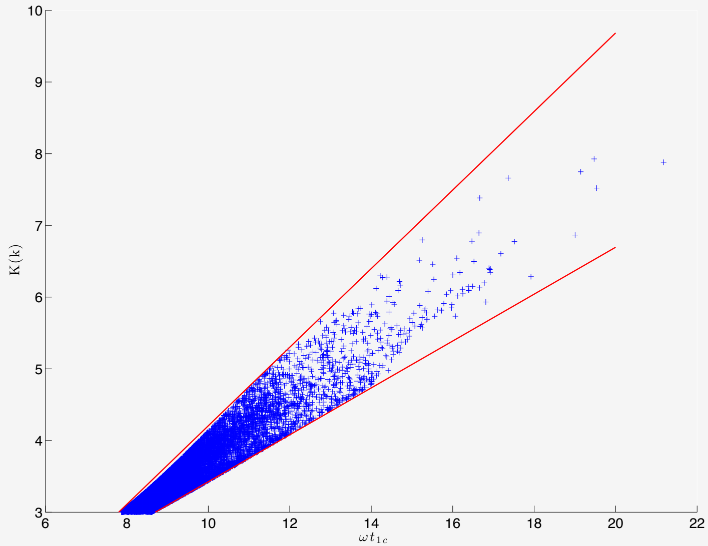


Family of simple loop strokes in the (x_1, x_2)-plane.

For several normal extremals parametrized by $\hat{p}(0)$, we compute the first conjugate time t_{1c} and the period of the strokes.



Oscillating case



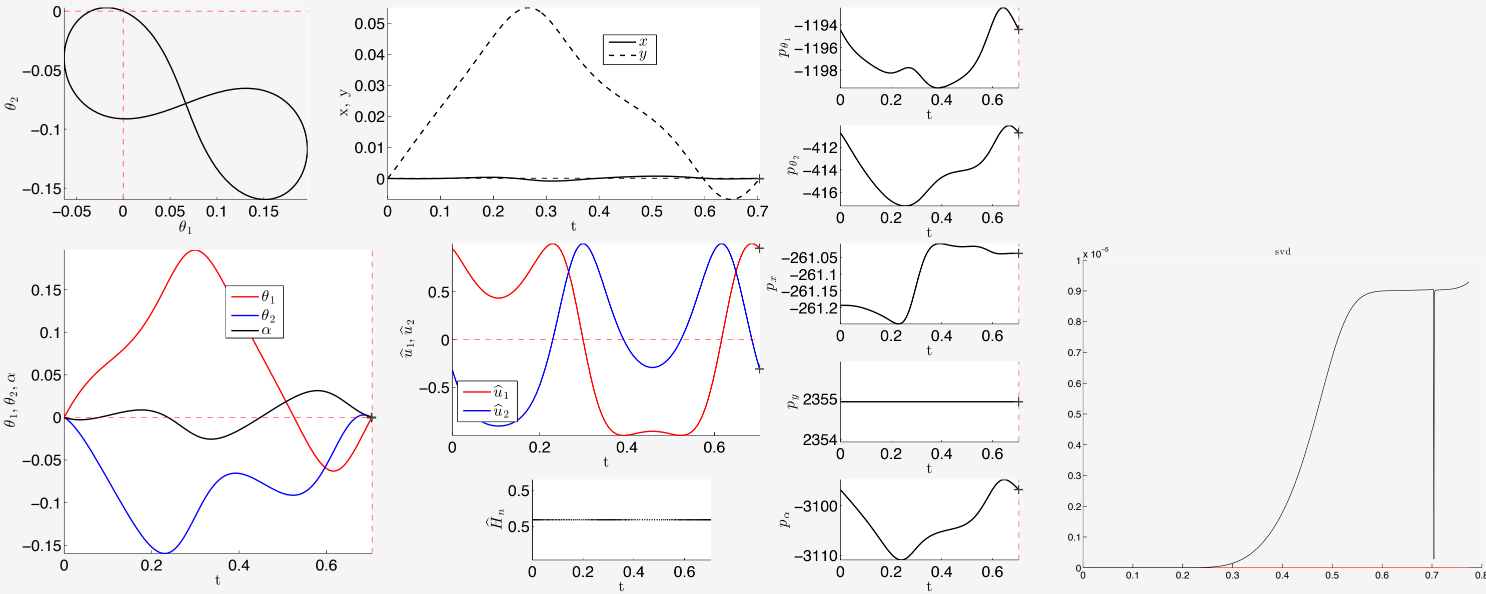
Rotating case

There is an affine dependance between the first conjugate time and the period of the strokes.

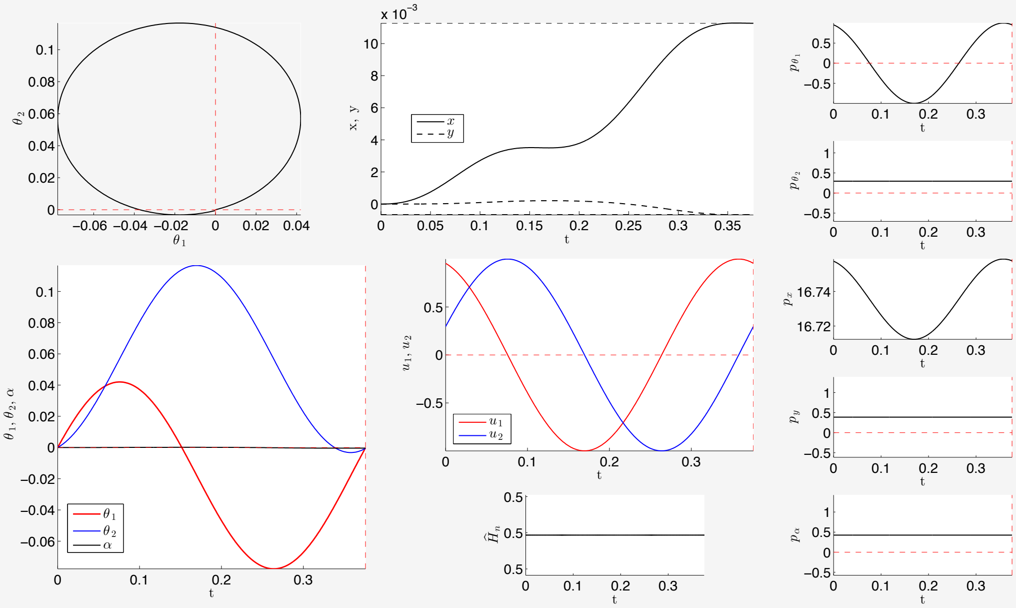
$$0.34\,\omega t_{1c} - 0.4 < K(k) < 0.53\,\omega t_{1c} - 0.8 \text{ for the oscillating case,}$$
$$0.33\,\omega t_{1c} + 0.16 < T < 0.55\,\omega t_{1c} - 1.27 \text{ for the rotating case.}$$

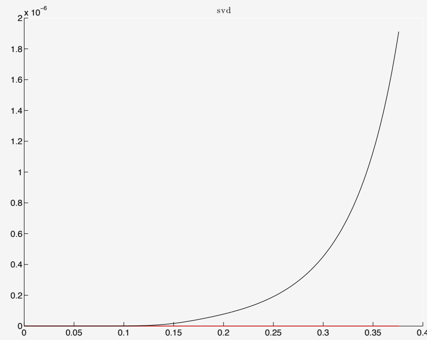
Theorem. *The normal extremal system associated with the nilpotent model is* **integrable** *and the solutions can be expressed as a polynomial functions of the first and the second order elliptic functions* $(u, \mathrm{sn}(u), \mathrm{cn}(u), \mathrm{dn}(u), E(u))$.

Simulations from analytical solutions.



(left) Control, state and adjoint physical variables in the oscillating case of the nilpotent approximation (eight shape). *(right)* SVD test of conjugate points.





(left) Control, state and adjoint physical variables in the rotating case of the nilpotent approximation $(k = 0.115)$. *(right)* SVD test of conjugate points.

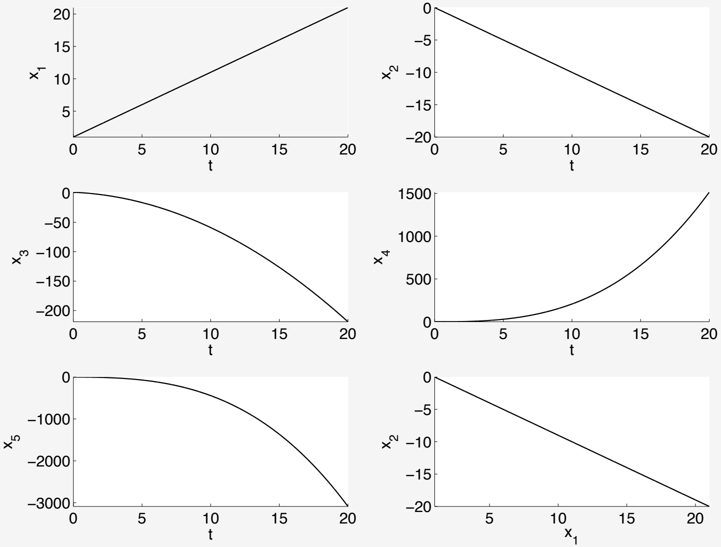
The simple loop strokes are candidate for optimality.

Theorem. *The system associated with abnormal extremals is* **integrable** *using polynomial functions.*

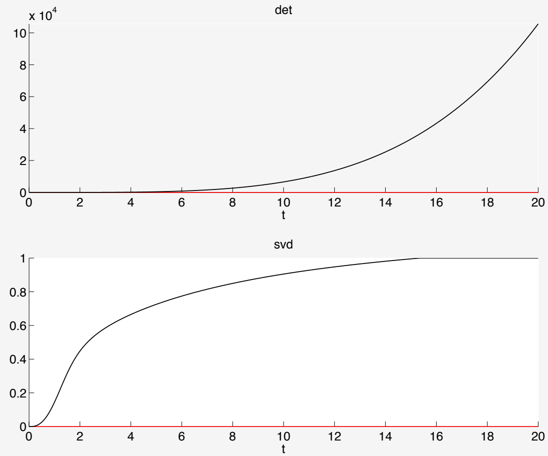
$$x_1(t) = t + x_{10},\; x_2(t) = 2\frac{p_{50}t}{p_{40}} + x_{20},\; x_3(t) = \frac{p_{50}t^2}{p_{40}} + 2\frac{p_{50}x_{10}t}{p_{40}} + x_{30},\; \ldots$$

$\Longrightarrow$ There are no abnormal smooth strokes for the nilpotent model.

Conjugate points



Optimal trajectory: state variables for the anormal case.



Second order sufficient condition for the anormal case checked with the determinant test and the smallest singular value associated with the rank condition.

- The nilpotent model gives an initialization for the shooting algorithm to compute **strokes with small amplitudes** on the real dynamic associated with the cost $\int_0^T u_1^2 + u_2^2 \mathrm{d}t$.

Boundary value problem

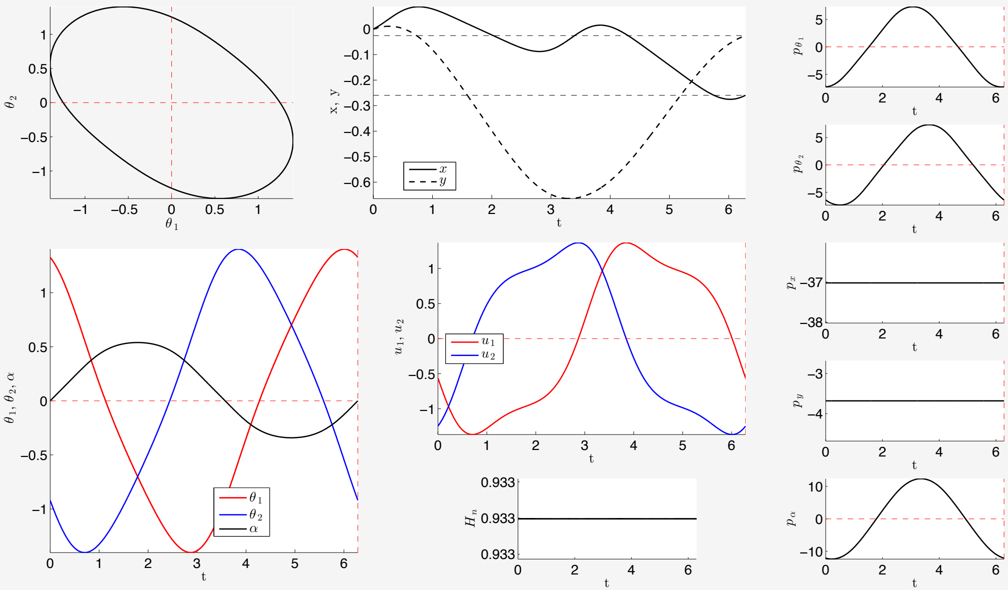
$$
\begin{cases}
\dot{q} = \frac{\partial \widetilde{H}_n}{\partial p}, \quad \dot{p} = -\frac{\partial \widetilde{H}_n}{\partial q}, \\
\theta_j(T) = \theta_j(0) \quad j = 1,2, \\
x(0) = y(0) = \alpha(0) = 0, \\
x(T)^2 + y(T)^2 = c_1, \, \alpha(T) = c_2, \\
p_{\theta_j}(T) = p_{\theta_j}(0) \quad j = 1,2, p_\alpha(0) = p_\alpha(T)
\end{cases}
$$

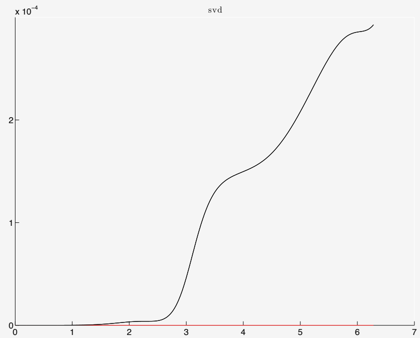
$\widetilde{H}_n$: normal Hamiltonian associated with the $\int_0^T (u_1^2 + u_2^2)\,\mathrm{d}t$ cost.

- We perform **two discrete homotopies**:
  - on c_1, to control the amplitude of the strokes,
  - on the cost (from the $\int_0^T u_1^2 + u_2^2 \,\mathrm{d}t$ cost to the mechanical cost).

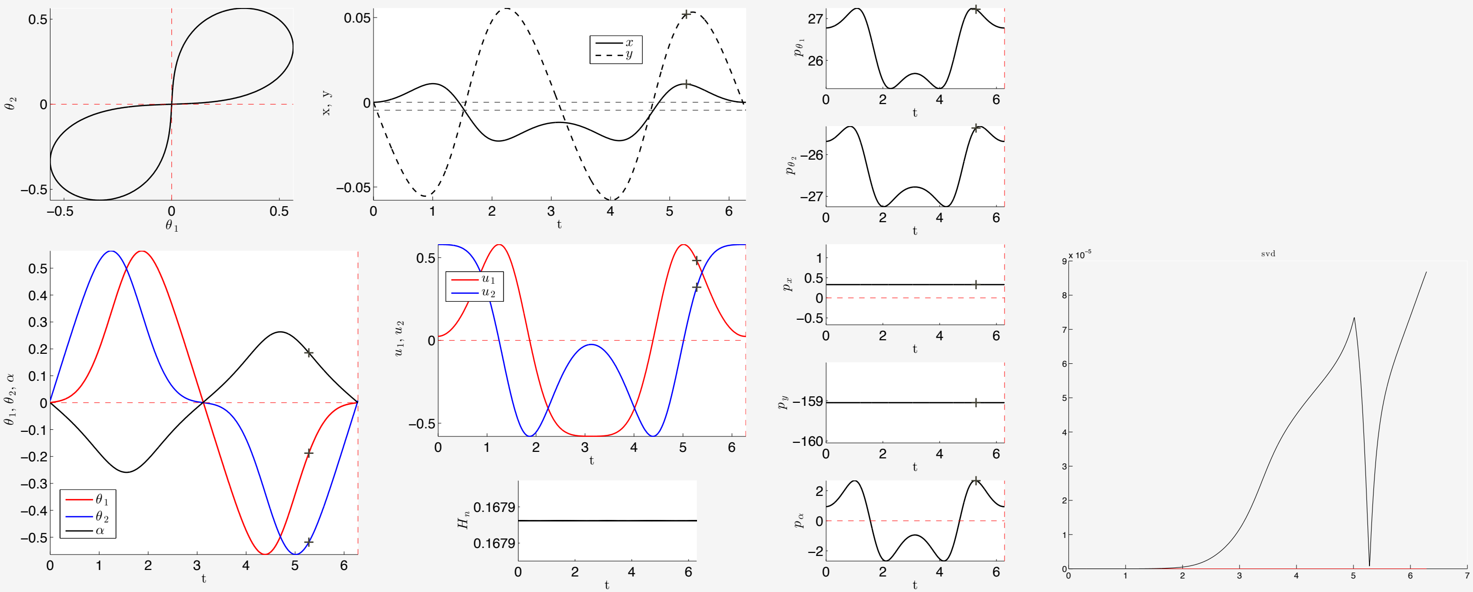
Strokes for the real dynamic with the $\int_0^T u_1^2 + u_2^2 \,\mathrm{d}t$ cost

Discrete homotopy on the amplitude of the strokes.





(left) Simple loop stroke for the Purcell swimmer minimizing the cost $\int_0^T (u_1^2 + u_2^2)\mathrm{d}t$, taking $T = 2\pi$, $c_1 = 0.068$, $c_2 = 0$ and imposing the periodicity on α. *(right)* Test of conjugate points (no conjugate point on $[0, 2\pi]$).



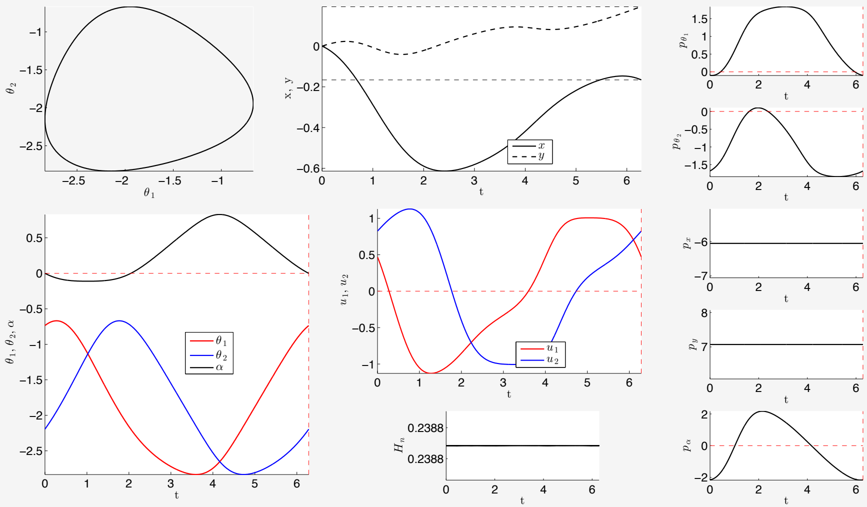
(left) Eight stroke for the Purcell swimmer minimizing the cost $\int_0^T (u_1^2 + u_2^2)\mathrm{d}t$, taking $T = 2\pi$, $c_1 = 4.6e{-}4$, $c_2 = 0$ and imposing the periodicity on α. *(right)* Test of conjugate points.

Discrete homotopy on the normal Hamiltonian.

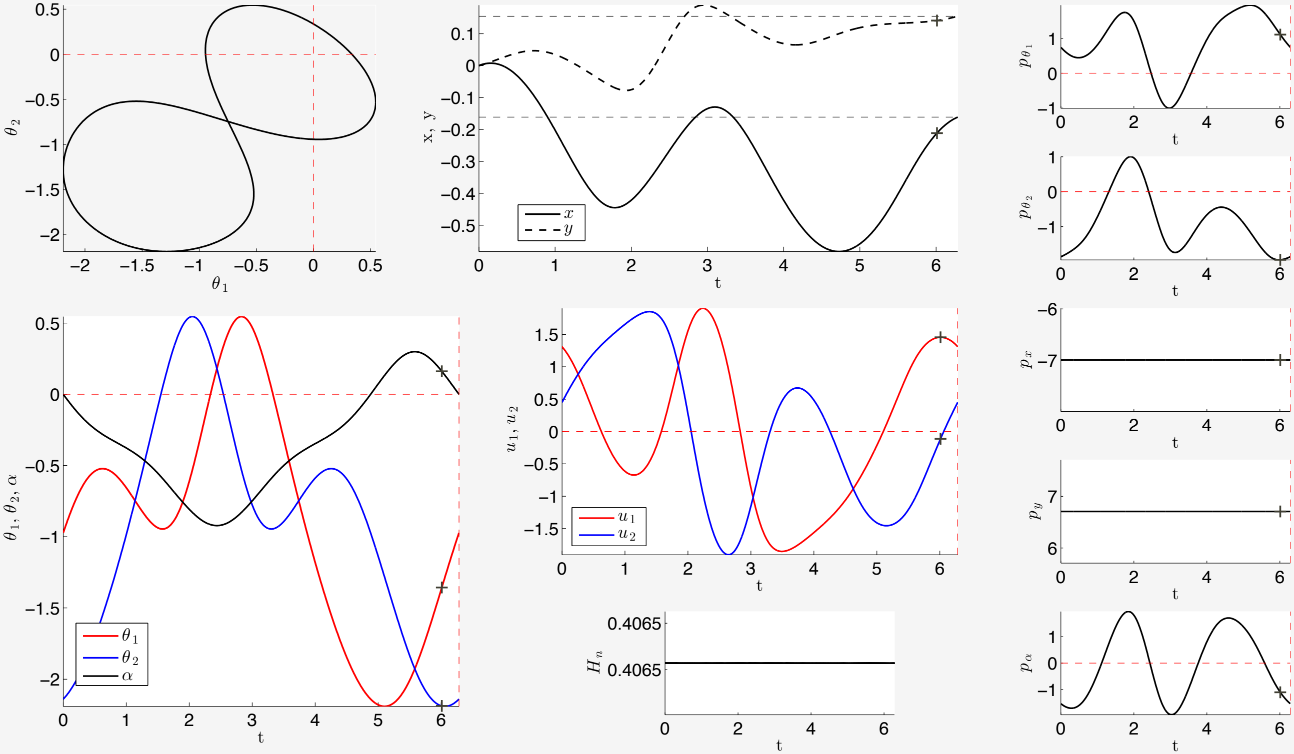
- $\widetilde{H}_n$: normal Hamiltonian of the real dynamic with the $\int_0^T u_1^2 + u_2^2 \mathrm{d}t$ **cost**,
- H_n: normal Hamiltonian of the real dynamic with the **mechanical cost**,

We consider

$$H = \lambda H_n + (1-\lambda)\widetilde{H}_n,\ \lambda \in [0,1].$$

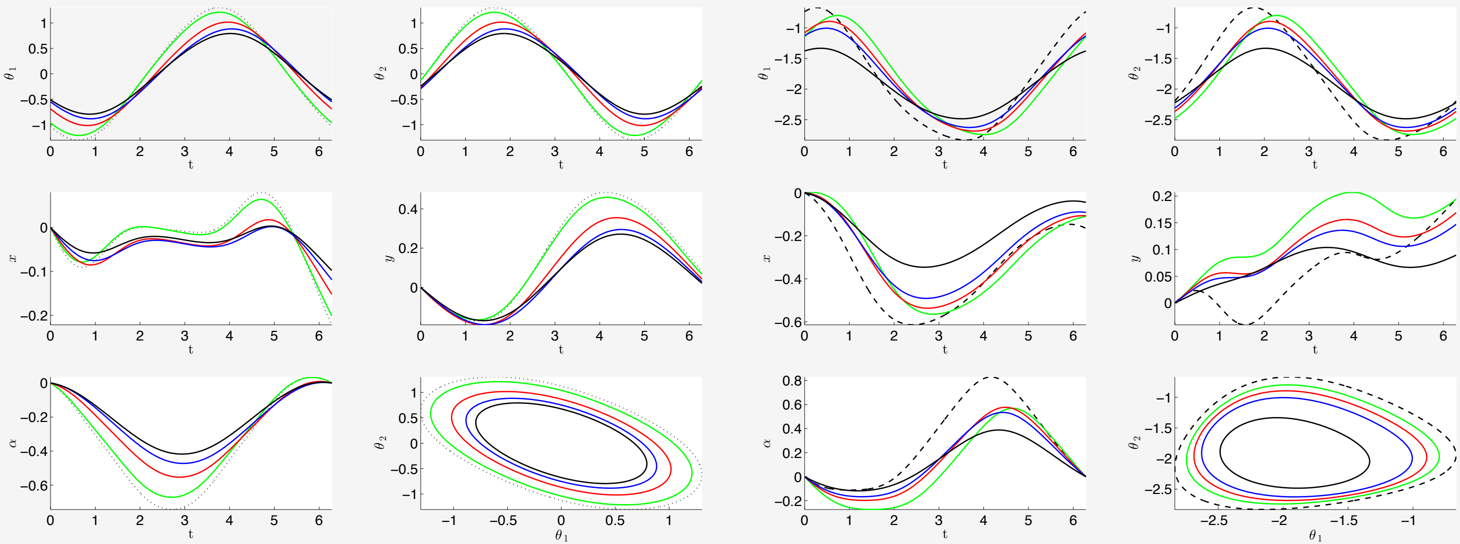


State and adjoint variables for the Purcell swimmer minimizing the mechanical cost, taking $T = 2\pi$, $c_1 = 0.065$ and $c_2 = 0$.



State and adjoint variables for the Purcell swimmer minimizing the mechanical cost, taking $T = 2\pi$, $c_1 = 0.05$ and $c_2 = 0$.

The differential homotopy fails due to the existence of several zeros curves. The discrete homotopy gives (at least) two families of strokes.



Families of simple loop strokes for the Purcell swimmer minimizing the mechanical cost.

Write the optimal control problem as

$$\begin{cases} \text{Minimize } J(q(.),u(.)) = \int_0^T L(q(t),u(t))\mathrm{d}t \\ \text{subject to} \\ \dot{x}(t) \; = \; F(q(t),u(t)) \quad \text{a.e. } t \in [0,T]\,, \\ u(t) \; \in \; U \quad \text{a.e. } t \in [0,T]\,, \\ c(q(0),q(T)) = 0\,, \end{cases}$$

and let $(\overline{q},\overline{p})$ **be an extremal solution** associated with the control u.
We consider the state transition matrix $\Phi(.,.)$ associated with the linearized Hamiltonian system

$$\begin{cases} \frac{\mathrm{d}}{\mathrm{d}t}\Phi(t,s) = Z\Phi(t,s) \\ \Phi(s,s) = \mathrm{Id}, \end{cases}$$

where

$$Z := \begin{bmatrix} \partial_q F - \partial_u F[\partial_{uu}H]^{-1}\partial_{qu}H^T & -\partial_u F[\partial_{uu}H]^{-1}\partial_u F^T \\ -\partial_{qq}H + \partial_{qu}H[\partial_{uu}H]^{-1}\partial_{qu}H^T & -\partial_q F[\partial_{uu}H]^{-1}\partial_u F^T \end{bmatrix}.$$

where H is the normal Hamiltonian (all matrices are evaluated along $(\overline{q},\overline{p})$).

The monodromy matrix is

$$W := \begin{bmatrix} \phi_{22}\phi_{12}^{-1} & \phi_{21} - \phi_{22}\phi_{12}^{-1}\phi_{11} \\ -\phi_{12} & \phi_{12}^{-1}\phi_{11} \end{bmatrix}, \quad \Phi(0,T) =: \begin{bmatrix} \phi_{11} & \phi_{12} \\ \phi_{21} & \phi_{22} \end{bmatrix}$$

Theorem (Standard conditions)**.** *Take a normal extremal for* $(q(.),u(.))$*. Suppose that*

(i) $R(t) > \varepsilon Id$ *on* $[0,T]$, $u(.)$ *bounded and* $(A(.),B(.))$ *is controllable on* $[0,T]$*,*

(ii): the extremal $(\overline{q}(.),\overline{u}(.),p(.))$ **doesn't have a conjugate point** *on* $[0,T]$*,*

(iii): there exists $\gamma > 0$ *such that*

$$[\xi_0^T \ \xi_1^T]\, W \begin{bmatrix} \xi_0 \\ \xi_1 \end{bmatrix} > \gamma \left\| \begin{bmatrix} \xi_0 \\ \xi_1 \end{bmatrix} \right\|^2,$$

for all vectors $\xi_0, \xi_1 \in \mathbb{R}^n \setminus \{0\}$ *satisfying*

$$D_{q_0}c((\overline{q}(0),\overline{q}(T)))\xi_0 + D_{q_T}c((\overline{q}(0),\overline{q}(T)))\xi_1 = 0.$$

Then $(\overline{q}(.),\overline{u}(.))$ *is a weak locally* **unique** *minimizer.*

Proposition. *Take* $a=(\phi,\sigma)\in I=(-\varepsilon,\varepsilon)^2$ *for some* $\varepsilon>0$. *Let* $\overline{q}=(\overline{\theta}_1,\overline{\theta}_2,\overline{x},\overline{y},\overline{\alpha})$ *a stroke associated with control* $\overline{u}=(\overline{u}_1,\overline{u}_2)$ *and adjoint vector* p. *For all* $a\in I$ *and* $t\in[0,T]$, *we define*

$$\begin{aligned}
&u_j^a(t)=\overline{u}_j(t+\sigma),\ \theta_j^a(t)=\overline{\theta}_j(t+\sigma) \quad j=1,2,\\
&x^a(t)=\cos(\phi)x^\sigma(t)+\sin(\phi)y^\sigma(t),\\
&y^a(t)=\sin(\phi)x^\sigma(t)-\cos(\phi)y^\sigma(t),\\
&\alpha^a(t)=\overline{\alpha}(t+\sigma)+\phi
\end{aligned}$$

where

$$\begin{aligned}
x^\sigma(t)&=\int_0^t\Big(u_1^a(s)F_{13}(\theta_1^a(s),\theta_2^a(s),\overline{\alpha}(s+\sigma))+u_2^a(s)F_{23}(\theta_1^a(s),\theta_2^a(s),\overline{\alpha}(s+\sigma))\Big)\mathrm{d}s,\\
y^\sigma(t)&=\int_0^t\Big(u_1^a(s)F_{14}(\theta_1^a(s),\theta_2^a(s),\overline{\alpha}(s+\sigma))+u_2^a(s)F_{24}(\theta_1^a(s),\theta_2^a(s),\overline{\alpha}(s+\sigma))\Big)\mathrm{d}s.
\end{aligned}$$

Then the normal extremal $(\overline{q}(.),p(.),\overline{u}(.))$ *is* **continuously embedded** *in the family of extremals* $(q^a(.),p^a(.),u^a(.))_{a\in I}$ *where* $p^a(.)$ *is the adjoint vector associated with* $(q^a(.),u^a(.))$.

$\Longrightarrow$ **The standard sufficient conditions necessary fail.**

Theorem (Refined conditions, Vinter). *Suppose that a weak normal extremal* $(\overline{q}(.), \overline{u}(.), p(.))$ *can be continuously embedded in a family of weak normal extremals, and that*

(i) $R(t) > \varepsilon Id$ *on* $[0,T]$, $u(.)$ *bounded and* $(A(.), B(.))$ *is controllable on* $[0,T]$,

(ii): the extremal $(\overline{q}(.), \overline{u}(.), p(.))$ **doesn't have a conjugate point** *on* $[0,T]$,

(iii): there exists $\gamma > 0$ *such that*

$$[\xi_0^T \ \xi_1^T] W \begin{bmatrix} \xi_0 \\ \xi_1 \end{bmatrix} > \gamma \left\| \begin{bmatrix} \xi_0 \\ \xi_1 \end{bmatrix} \right\|^2 ,$$

for all vectors $\xi_0, \xi_1 \in \mathbb{R}^n \setminus \{0\}$ *satisfying*

$$D_{q_0} c((\overline{q}(0), \overline{q}(T)))\xi_0 + D_{q_T} c((\overline{q}(0), \overline{q}(T)))\xi_1 = 0 \qquad \text{and} \qquad \Gamma^T \begin{bmatrix} \xi_0 \\ \xi_1 \end{bmatrix} = 0 .$$

where $\Gamma := \begin{bmatrix} D_\alpha q^\alpha(0) \\ D_\alpha q^\alpha(T) \end{bmatrix} \Bigg|_{\alpha=0}$.

Then $(\overline{q}(.), \overline{u}(.))$ *is a* **weak local minimizer**.

Numerical results

Monodromy matrix. Numerical integration (*lsoda* from *odepack* library) yields:

$$
W = \begin{pmatrix}
36.7491 & -12.3797 & -90.3501 & -38.4486 & 45.9572 & -20.9543 & 12.3334 & 90.3501 & 38.4486 & -22.0849 \\
-12.3797 & 12.7351 & 63.8598 & -2.19107 & -4.48021 & 5.29771 & -14.0060 & -63.8598 & 2.19107 & -7.52291 \\
-90.3501 & 63.8598 & 356.119 & 72.4282 & -72.3005 & 50.6364 & -65.6286 & -356.119 & -72.4282 & 5.46840 \\
-38.4486 & -2.19107 & 72.4283 & 155.119 & -58.0160 & 27.2663 & -1.54193 & -72.4283 & -155.119 & 30.3765 \\
45.9572 & -4.48021 & -72.3005 & -58.0160 & 74.6500 & -29.6527 & 3.10041 & 72.3005 & 58.0160 & -51.0282 \\
-20.9543 & 5.29771 & 50.6364 & 27.2663 & -29.6527 & 11.6627 & -5.47480 & -50.6364 & -27.2663 & 15.3254 \\
12.3334 & -14.0060 & -65.6286 & -1.54192 & 3.10041 & -5.47479 & 15.7573 & 65.6286 & 1.54192 & 9.86428 \\
90.3501 & -63.8598 & -356.119 & -72.4282 & 72.3005 & -50.6364 & 65.6286 & 283.095 & 72.4282 & -5.46840 \\
38.4486 & 2.19107 & -72.4283 & -155.119 & 58.0160 & -27.2663 & 1.54193 & 72.4283 & 82.0946 & -30.3765 \\
-22.0850 & -7.52291 & 5.46840 & 30.3766 & -51.0282 & 15.3254 & 9.86428 & -5.46840 & -30.3766 & 44.9320
\end{pmatrix}.
$$

Aim: Check that the standard conditions fail and the refined ones are satisfied $\Longrightarrow$ check the positiveness of W on appropriate subspaces.

We set

$$\mathscr{L}_1 = \{\, (y_0, y_T) \in \mathbb{R}^5 \times \mathbb{R}^5 \mid \nabla_{q_0,q_T} c(q_0, q_T)\, (y_0 \quad y_T)^\intercal = 0 \,\}$$

where

$$c(q_0, q_T) = \begin{pmatrix} \theta_1(0) - \theta_1(T) \\ \theta_2(0) - \theta_2(T) \\ x(0) \\ y(0) \\ \alpha(0) - \alpha(T) \\ x(T)^2 + y(T)^2 - r \end{pmatrix}.$$

Define the matrix N_1 such that $\ker(\nabla_{q_0,q_T} c(q_0, q_T)) = \mathrm{Im}(N_1)$.

Standard conditions. Is the matrix $\widetilde{W}_1 = N_1^\intercal (W^\intercal + W) N_1$ positive-definite?

Define the matrices

$$\Gamma_\phi = \begin{pmatrix} \nabla_\phi q^a(0) \\ \nabla_\phi q^a(T) \end{pmatrix}_{\phi=0}, \; \Gamma_\sigma = \begin{pmatrix} \nabla_\sigma q^a(0) \\ \nabla_\sigma q^a(T) \end{pmatrix}_{\sigma=0} \text{ and } \widehat{\Gamma} = \begin{pmatrix} \Gamma_\phi & \Gamma_\sigma \end{pmatrix}.$$

and the linear subspaces

$$\mathscr{L}_\phi = \mathscr{L}_1 \cap \{(y_0, y_T) \in \mathbb{R}^5 \times \mathbb{R}^5 \mid \Gamma_\phi^\intercal \begin{pmatrix} y_0 & y_T \end{pmatrix}^\intercal = 0\},$$
$$\mathscr{L}_\sigma = \mathscr{L}_1 \cap \{(y_0, y_T) \in \mathbb{R}^5 \times \mathbb{R}^5 \mid \Gamma_\sigma^\intercal \begin{pmatrix} y_0 & y_T \end{pmatrix}^\intercal = 0\},$$
$$\widehat{\mathscr{L}} = \mathscr{L}_1 \cap \{(y_0, y_T) \in \mathbb{R}^5 \times \mathbb{R}^5 \mid \widehat{\Gamma}^\intercal \begin{pmatrix} y_0 & y_T \end{pmatrix}^\intercal = 0\}$$

and the matrices N_ϕ, N_σ and $\widehat{N}$ such that

$$\mathscr{L}_\phi = \mathrm{Im}(N_\phi), \quad \mathscr{L}_\sigma = \mathrm{Im}(N_\sigma), \quad \widehat{\mathscr{L}} = \mathrm{Im}(\widehat{N}).$$

Refined conditions. Is the matrix $\widehat{W} = \widehat{N}^\intercal (W^\intercal + W)\widehat{N}$ positive-definite?

Absolute and relative tolerance	(Standard condition) $\mathrm{Spec}(\widetilde{W}_1)$	$\mathrm{Spec}(\widetilde{W}_\phi)$	$\mathrm{Spec}(\widetilde{W}_\sigma)$	(Refined condition) $\mathrm{Spec}(\widehat{W})$
$\sim 10^{-4}$	1319.91 3.44629 -2.61575×10^{-5} -4.17860×10^{-3}	35380.1 3.46392 -4.18945×10^{-3}	1366.83 -4.10573×10^{-4} 14.5123	36179.7 13.8018
$\sim 10^{-7}$	1320.17 3.44676 9.81190×10^{-6} -5.40128×10^{-6}	35386.9 3.46438 -4.84724×10^{-6}	1367.10 9.85195×10^{-6} 14.5151	36186.9 13.8037

- The standard condition failed: $\widetilde{W}_1$ has zero eigenvalues.
- The refined condition is satisfied: $\widehat{W}$ is positive-definite.
- The matrices $\widetilde{W}_\phi = N_\phi^\intercal (W^\intercal + W) N_\phi$ and $\widetilde{W}_\sigma = N_\sigma^\intercal (W^\intercal + W) N_\sigma$ have zero eigenvalues (whose eigenvectors are Γ_ϕ and Γ_σ).

Theorem. *The simple loop $(\overline{q}, \overline{u})$ is weak-locally optimal.*