Geometric optimal control for microorganisms

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MODE-SMAI 2016, 23th March

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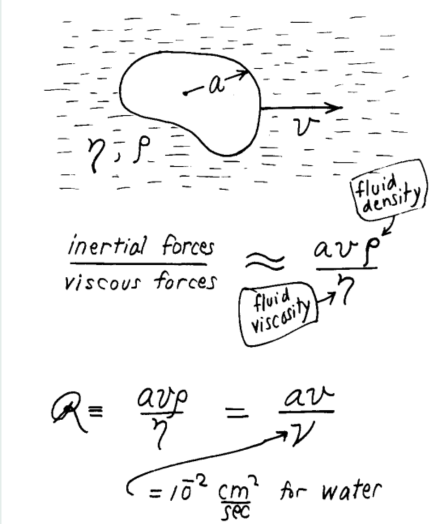
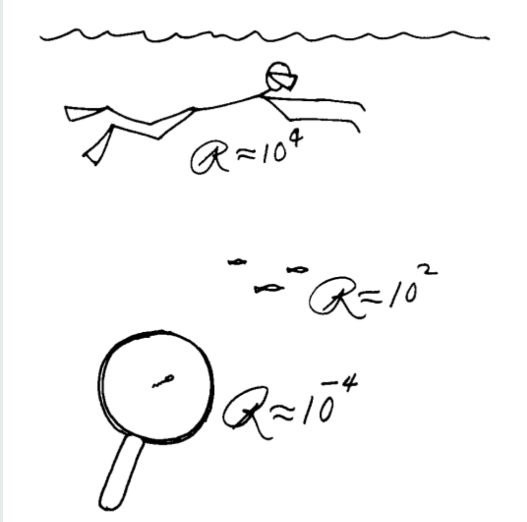
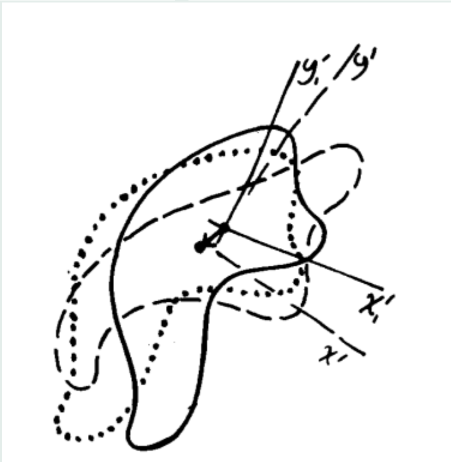
Life at low Reynolds number (Purcell, 1977)



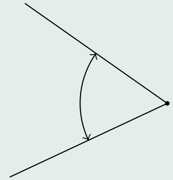




Shape deformations of a microswimmer

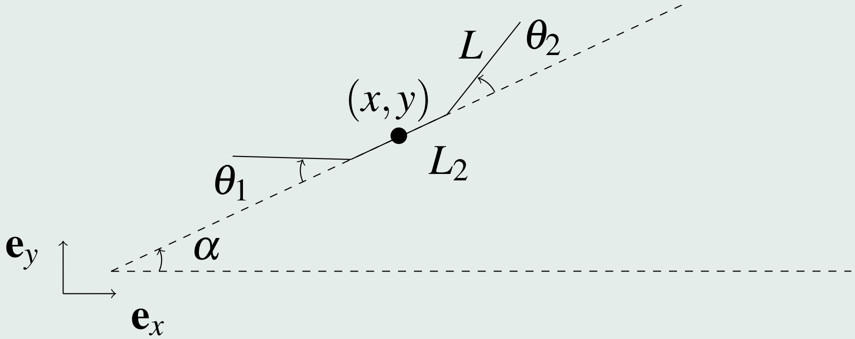
The Purcell Three-link swimmer

Two-link swimmer: a scallop.



Theorem. *A scallop cannot swim.*

Three-link swimmer: the Purcell swimmer.



Dynamics.

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

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

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

Purcell: mathematical model

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

Mechanical nonholonomic system.

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

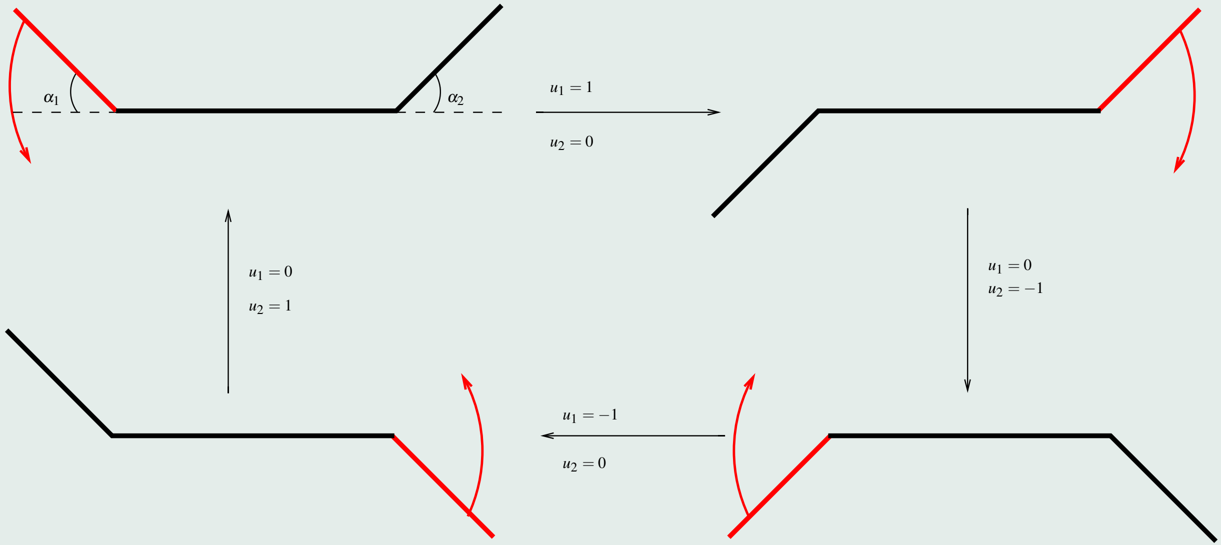
Sub-Riemannian geometry. (M, D, g) where M is an $n-$dimensional manifold, D a distribution of constant rank $m \leq n$ and g is a Riemannian metric on D.
$D_1 = \mathrm{span}\{F_1, F_2\}$, $D_2 = D_1 \cup \mathrm{span}\{[F_1, F_2]\}$, $D_3 = D_2 \cup \mathrm{span}\{[[F_1, F_2], F_1], [[F_1, F_2], F_2]\}$.
At a point X_0, $D_1(X_0)$ is a $(2, 3, 5)-$distribution.

- compute the **nilpotent approximation** of the Purcell swimmer
- consider a simplified model: **Copepod swimmer**

Find closed projections of geodesics.

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 $T = 2\pi$).*

Example of a Purcell stroke.



The displacement associated with the sequence stroke is

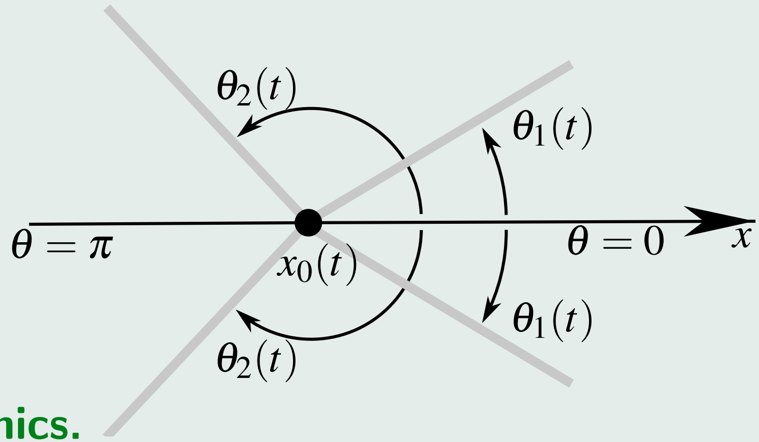
$$\beta(t) = (\exp tF_2 \ \exp -tF_1 \ \exp -tF_2 \ \exp tF_1)(X(0))$$

and using Baker-Campbell-Hausdorff formula

$$\beta(t) = \exp(t^2[F_1, F_2] + o(t^2))(X(0)) \sim X(0) + t^2[F_1, F_2](X(0))$$

Copepod swimmer (Takagi, 2014)

Symmetric model of swimming of an abundant variety of zooplankton.
Aim: **Build a micro swimmer** device (contact Takagi).



Controlled dynamics.

$$\dot{x}_0 = \frac{u_1 \sin(\theta_1) + u_2 \sin(\theta_2)}{2 + \sin^2(\theta_1) + \sin^2(\theta_2)}, \quad \dot{\theta}_1 = u_1, \quad \dot{\theta}_2 = u_2 \quad (\text{constraint: } 0 \le \theta_1 \le \theta_2 \le \pi).$$

Minimize the Mechanical energy. $\dot{q} M \dot{q}^t$ where $q = (x_0, \theta_1, \theta_2)$ and M is the symmetric matrix

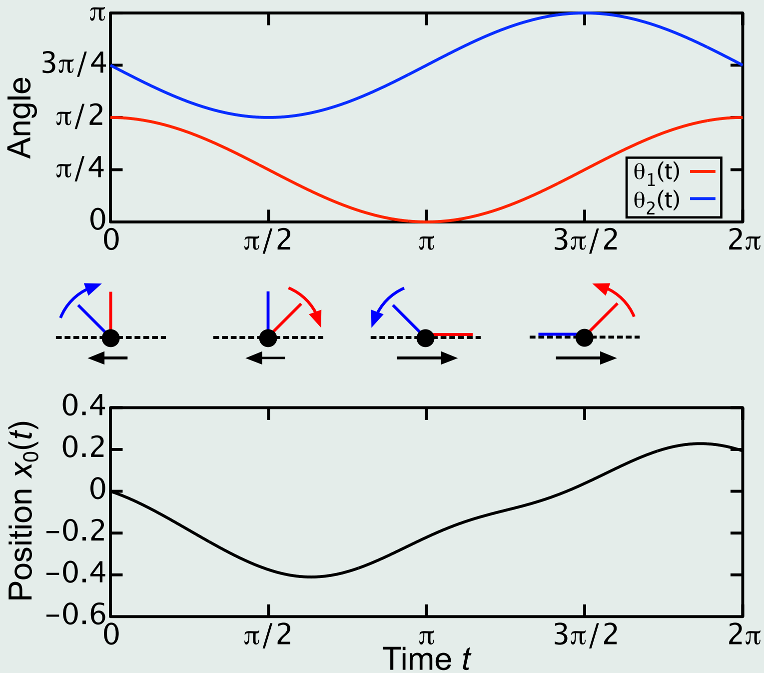
$$M = \begin{pmatrix} 2 - 1/2(\cos^2(\theta_1) + \cos^2(\theta_2)) & -1/2 \sin(\theta_1) & -1/2 \sin(\theta_2) \\ -1/2 \sin(\theta_1) & 1/3 & 0 \\ -1/2 \sin(\theta_2) & 0 & 1/3 \end{pmatrix}$$

Two types of geometric motions

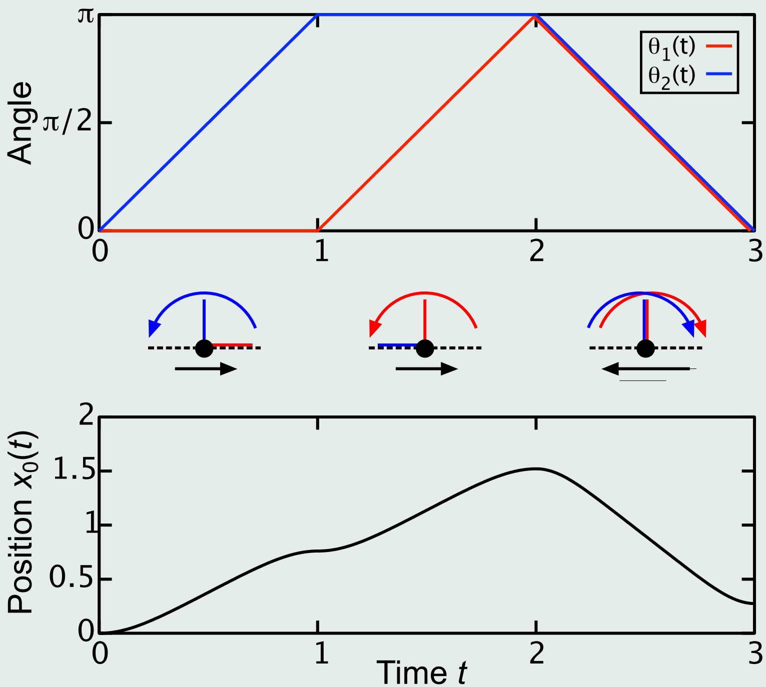
First case: The two legs are assumed to **oscillate sinusoidally** according to

$$\theta_1 = \Phi_1 + a\cos(t), \quad \theta_2 = \Phi_2 + a\cos(t + k_2)$$

with $a = \pi/4$, $\Phi_1 = \pi/4$, $\Phi_2 = 3\pi/4$ and $k_2 = \pi/2$. This produces a displacement $x_0(2\pi) = 0.2$.



Second case: The two legs are paddling in sequence followed by a recovery stroke performed in **unison**. In this case the controls $u_1 = \dot{\theta}_1$, $u_2 = \dot{\theta}_2$ produce bang arcs to steer the angles between from the boundary 0 of the domain to the boundary π, while the unison sequence corresponds to a displacement from π to 0 with the constraint $\theta_1 = \theta_2$.



Normal and Abnormal curves

- The driftless control system is

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

where $q = (x_0, \theta_1, \theta_2)$, $F_i = \frac{\sin(\theta_i)}{\Delta}\frac{\partial}{\partial x_0} + \frac{\partial}{\partial \theta_i}$ 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 $H(z, p^0, u) = u_1 H_1(z) + u_2 H_2(z) + p^0(u_1^2 + u_2^2)$

- Two types of extremals:

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

$$H_n = \frac{1}{2}(H_1^2 + H_2^2).$$

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

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

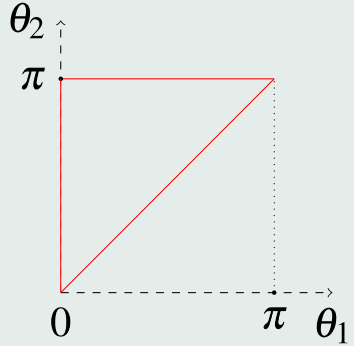
$$u_1 \{\{H_1, H_2\}, H_1\}(z) + u_2 \{\{H_1, H_2\}, H_2\}(z) = 0.$$

Computations for the copepod swimmer.

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

- $\theta_{1|2} = 0$ *or* π,
- $\theta_1 = \theta_2$.

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



: abnormal curve

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

Analysis outside the singular set Σ

$H_3 = \langle p, F_3(q)\rangle$, 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.

$$\dot{H}_1 = dH_1(\overrightarrow{H}_n) = \{H_1, H_2\}H_2 = H_2H_3,$$
$$\dot{H}_2 = dH_2(\overrightarrow{H}_n) = \{H_2, H_1\}H_1 = -H_1H_3,$$
$$\dot{H}_3 = dH_3(\overrightarrow{H}_n) = \{H_3, H_1\}H_1 + \{H_3, H_2\}H_2$$

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.**

Numerical results

Applying the PMP, we solve numerically boundary value problem:

$$\begin{cases} \dot{q} = \frac{\partial H_n}{\partial p}, \qquad \dot{p} = -\frac{\partial H_n}{\partial q}, \\ x_0(0) = 0, \quad x_0(2\pi) = x_f, \\ \theta_{1|2}(0) = \theta_{1|2}(2\pi), \quad p_{2|3}(0) = p_{2|3}(2\pi). \end{cases}$$

where H_n is the true Hamiltonian in the normal case

$$H_n = \frac{1}{2}\left(H_1^2 + H_2^2\right).$$

Two softwares used:

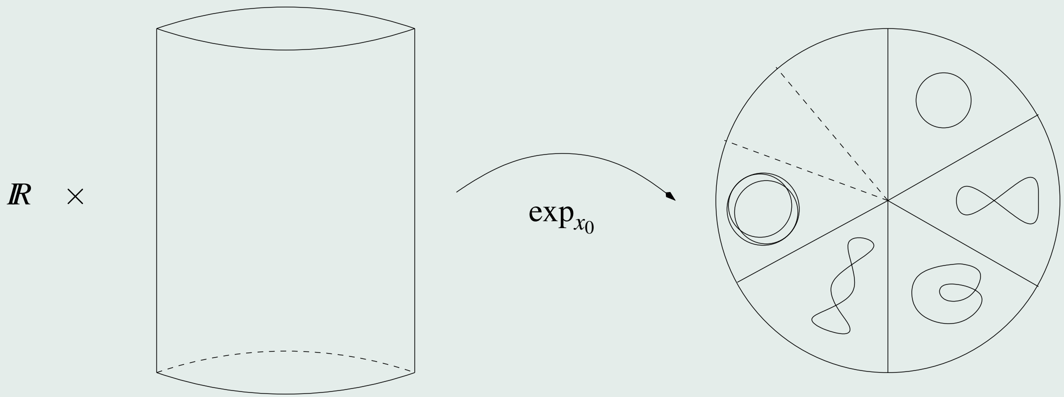
- `Bocop` (*direct method*: discretization of the state and control spaces $\rightarrow$ NLP problem) gives an initialisation for the shooting algorithm of the `HamPath` software.
- `HamPath` (*indirect method*: shooting algorithm, homotopic methods) compute a normal stroke and **second order optimality conditions**.

Exponential mapping

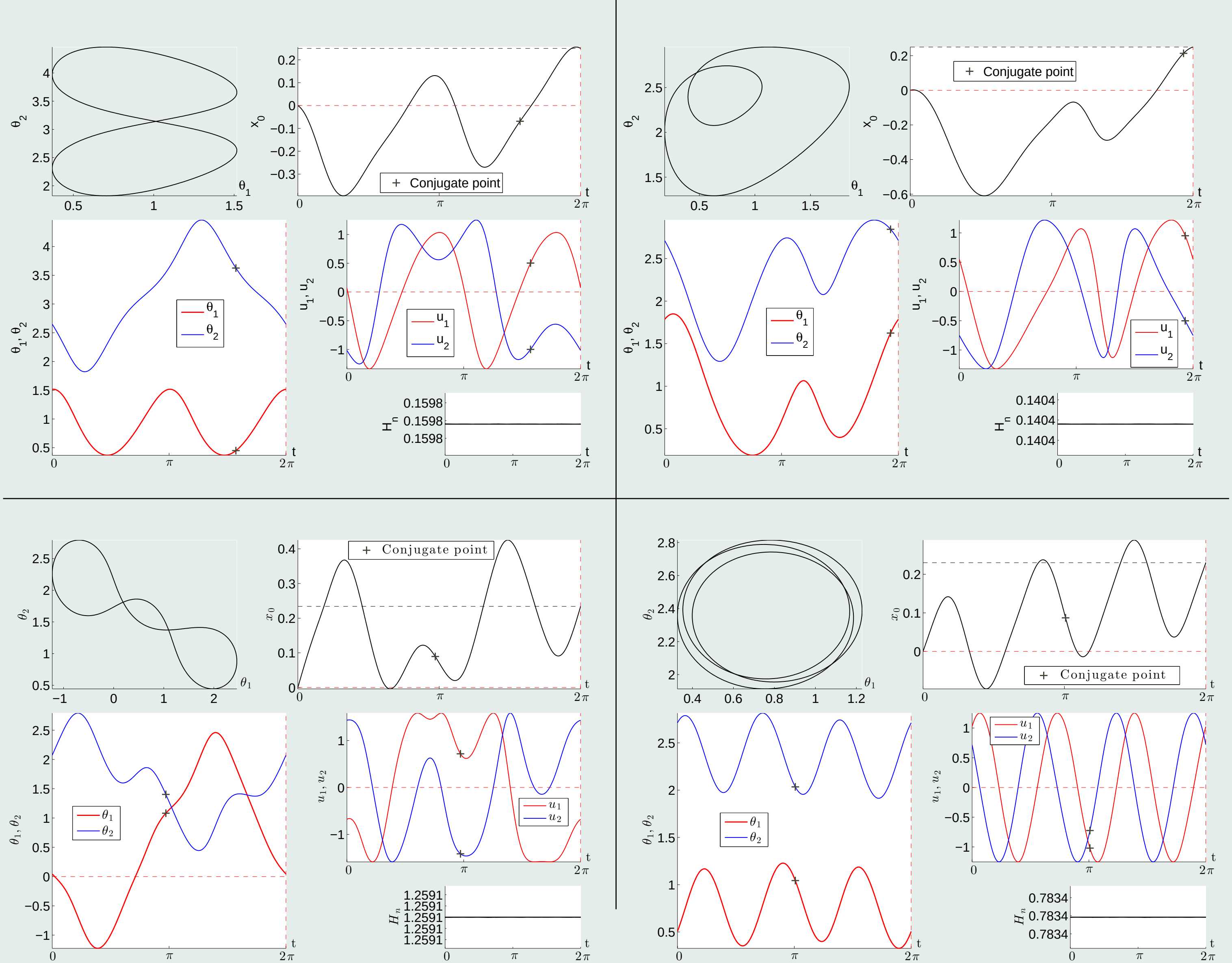
First conjugate time t_c: the exponential map

$$\exp_{x_0} : \mathbb{R} \times \mathscr{C} \to M, \quad (t, p_0) \mapsto x(t, x_0, p_0)$$

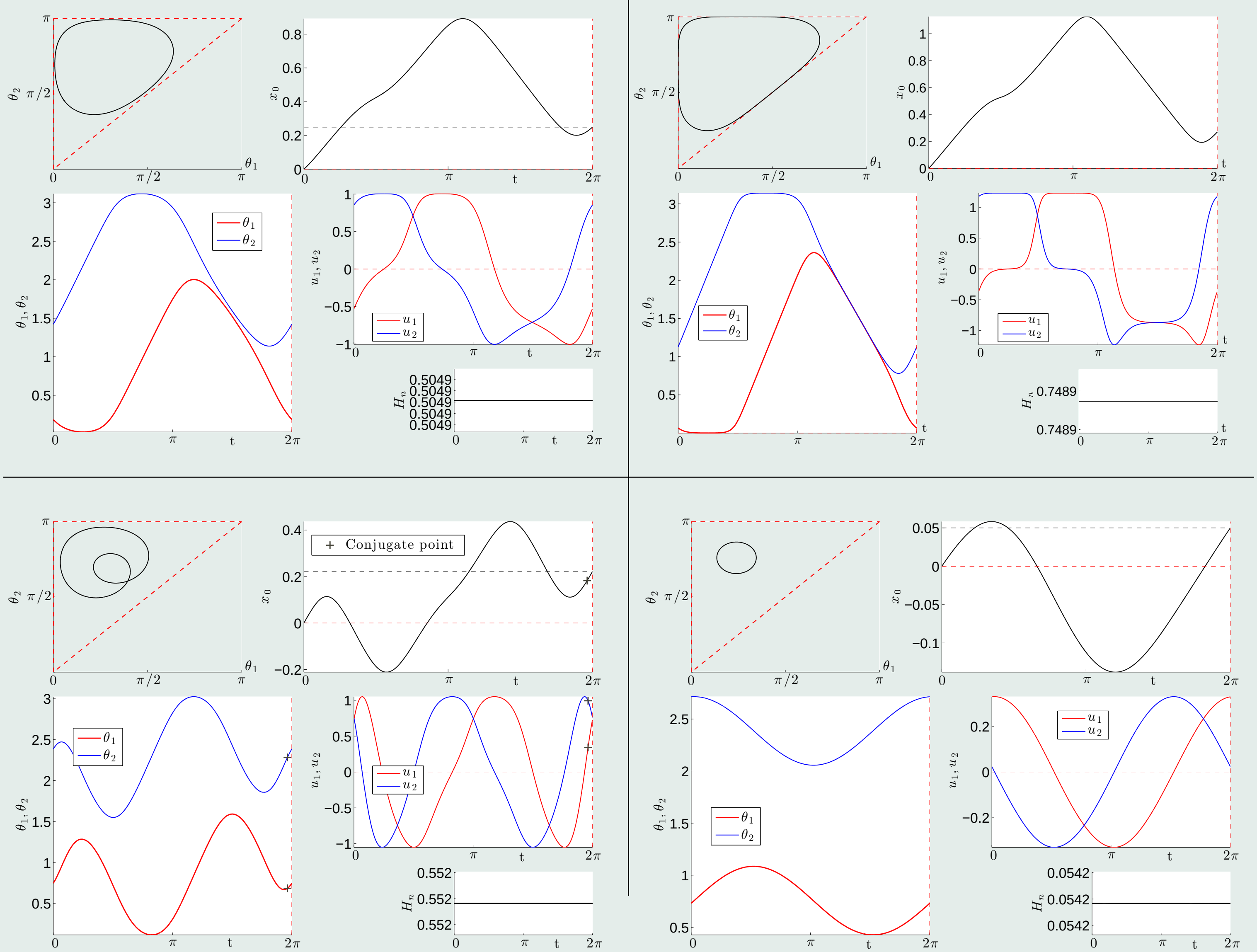
is not immersive at (t_c, p_0).
After t_c, the normal geodesic ceases to be minimizing with respect to the C^1-topology.



$$\mathscr{C} = \{ p_0 \mid H_1^2(x_0, p_0) + H_2^2(x_0, p_0) = 1 \}$$



Conjugate point
Conjugate point
Conjugate point
Conjugate point
θ_1
θ_2
x_0
u_1, u_2
θ_1, θ_2
H_n
t
0
π
2π
0.1598
0.1404
1.2591
0.7834



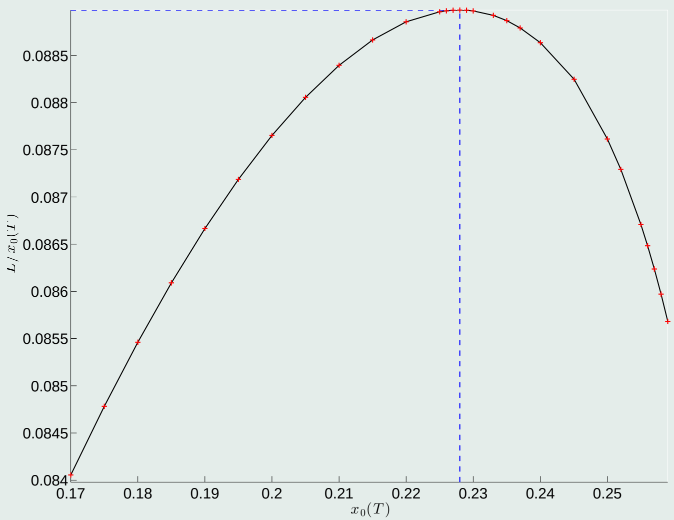
θ_1
θ_2
$\pi/2$
π
x_0
t
2π
θ_1, θ_2
u_1, u_2
u_1
u_2
H_n
0.5049
0.7489
0.552
0.0542
+ Conjugate point

Comparisons of strokes

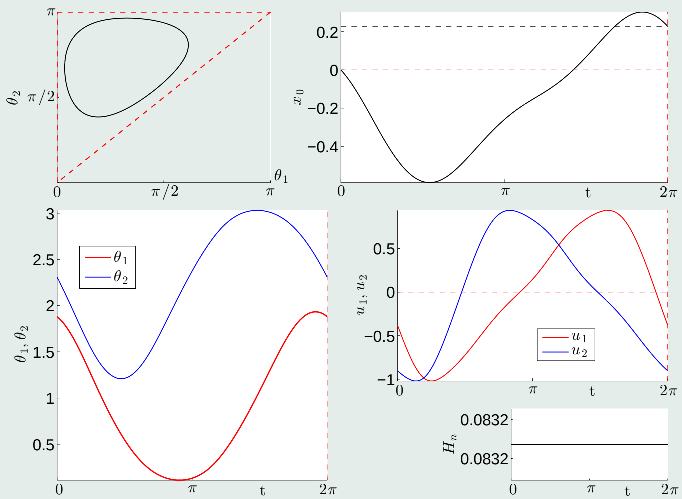
The **geometric efficiency** of a stroke γ is defined by the ratio $\boldsymbol{x_0/L(\gamma)}$,

- $L(\gamma)$ is the length of the stroke γ (*independent of the time parameterization*),
- x_0 the corresponding displacement.

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



Curves of efficiencies obtained by continuation on $x_0(T)$.



Stroke corresponding to the maximum of efficiency.

Conclusion about the Copepod swimmer

- Complex politics: classification of periodic planar curves.
- **Simple loops are the only candidates**.
- The abnormal triangle is not optimal due to the existence of corners.
- Concept of geometric efficiency.

Perspectives:

- Maximum Principle with state constraints.
- Compute the global optimum $\rightarrow$ related to count the number of strokes on each energy level.
- Micro swimmer devices with Takagi.

Nilpotent Approximation in SR Geometry

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.

Nilpotent Approximation for the Purcell

Theorem. *The nilpotent approximation at zero is*

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

Remark. *We have $\varphi \in \mathrm{Diff}(M)$ acting on F_i such that:*

$$(\varphi * F_1)(x) = \hat{F}_1(x), \ (\varphi * F_2)(x) = \hat{F}_2(x).$$

$\theta_1 = x_1$ *and* $\theta_2 = x_2$ *are invariant by the* φ*.*

Theorem. *1. The system associated to normal extremals is* **integrable** *and the solutions can be expressed as a polynomial functions of the first and the second order elliptic functions* $(u, \mathrm{sn}(u), \mathrm{cn}(u), \mathrm{dn}(u), E(u))$*,*

2. The system associated to anormal extremals is **integrable** *using polynomial functions.*

Normal extremals

Hamiltonian lifts.

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

SR problem.

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

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

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

We consider Poincaré coordinates

$$\dot{H}_1 = dH_1(\overrightarrow{H}) = \{H_1, H_2\}H_2 = \langle p, [\hat{F}_1, \hat{F}_2](x)\rangle H_2 = H_2H_3,$$

$$\begin{aligned} &\dot{H}_2 = -H_3H_1, && \dot{H}_3 = H_1H_4 + H_2H_5, \\ &\dot{H}_4 = 0 \quad \text{hence} \quad H_4 = c_4, && \dot{H}_5 = 0 \quad \text{hence} \quad H_5 = c_5. \end{aligned}$$

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

$$\dot{H}_1 = -\sin(\theta)\dot{\theta} = H_2H_3 = \sin(\theta)H_3.$$

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

$$\ddot{\theta} = -(H_1c_4 + H_2c_5) = -c_4\cos(\theta) - c_5\sin(\theta) = -\omega^2\sin(\theta + \phi)$$

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

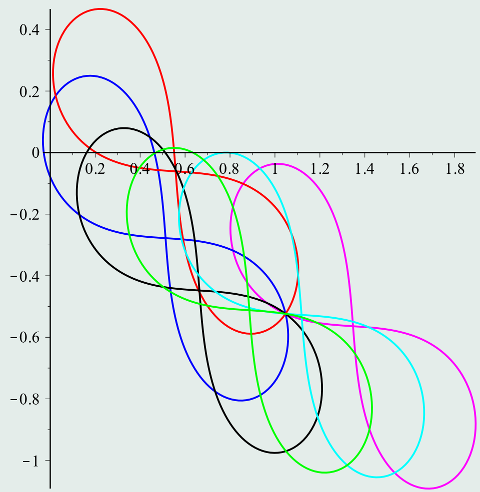
$$\frac{1}{2}\dot{\psi}^2 - \omega^2\cos(\psi) = B,$$

where B is a constant.

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

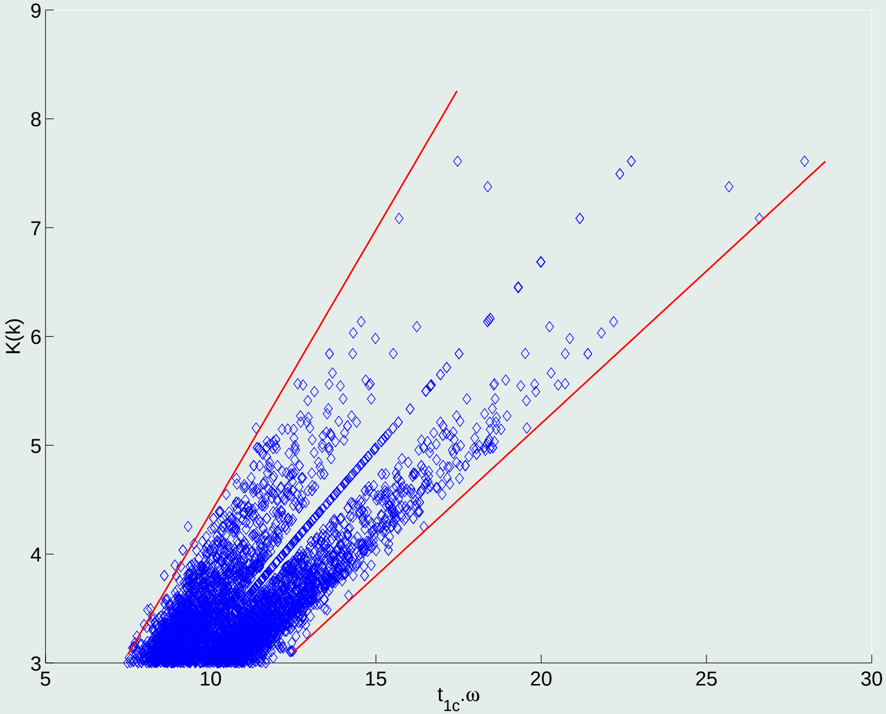
$$x_1(u) = \frac{1}{\omega}\Big[x_1(\varphi_0) - 2k\sin(\phi)\,\mathrm{cn}(u,k) + (-u + 2E(u,k))\cos(\phi)\Big],$$
$$x_2(u) = \frac{1}{\omega}\Big[x_2(\varphi_0) - 2k\cos(\phi)\,\mathrm{cn}(u,k) + (u - 2E(u,k))\sin(\phi)\Big],$$
$$x_3(u)\ldots, x_4(u)\ldots, x_5(u)\ldots$$

Family of strokes of **period $4K(k)/\omega$** (dependance on initial conditions $(x(0), p(0))$.



Family of eight shape strokes

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



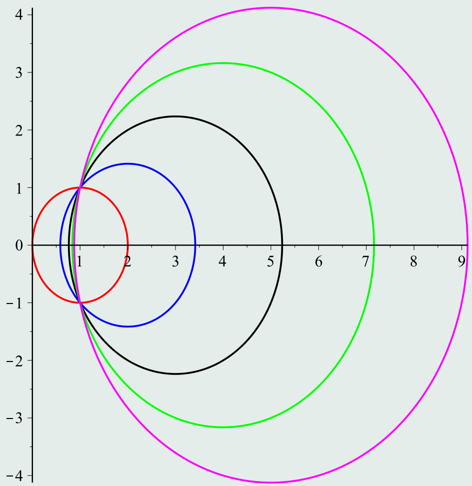
There is an affine dependance between the first conjugate time and the period of the strokes.

$$0.3\omega t_{1c} - 0.4 < K(k) < 0.5\omega t_{1c} - 0.8$$

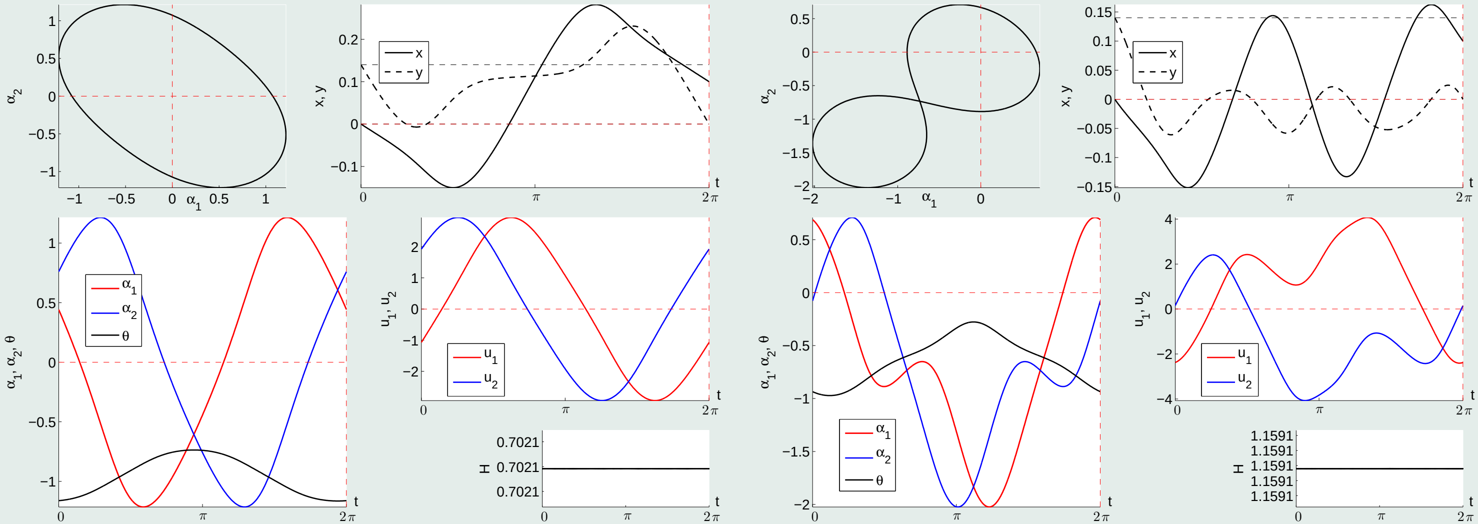
Rotating case.

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

Family of strokes of **period $2\pi/\omega$**.



Numerical simulations on the real system



Non self-intersecting and 8 solutions. There is no conjugate time $t_{1c} \in [0, 2\pi]$.

Extremals with the same cost

Symmetry with respect to θ_0.

Lemma. *If* $\theta(t)$, $\alpha(t)$, $\bar{x}(t)$, $\bar{y}(t)$ *is an extremal solution associated to* $u(.)$ *with* $\theta(0) = 0$, *then*

$$x(t) = \cos(\alpha_0)\bar{x}(t) - \sin(\alpha_0)\bar{y}(t),$$
$$y(t) = \sin(\alpha_0)\bar{x}(t) + \cos(\alpha_0)\bar{y}(t)$$

is the solution associated with $u(.)$ *with* $\alpha(0) = \alpha_0$, $(x(0), y(0)) = (\bar{x}_0, \bar{y}_0)$ *and with the same cost.*

Standard second order sufficient conditions.

- local minimizer for L^∞-topology
- this extremum is **locally unique**.

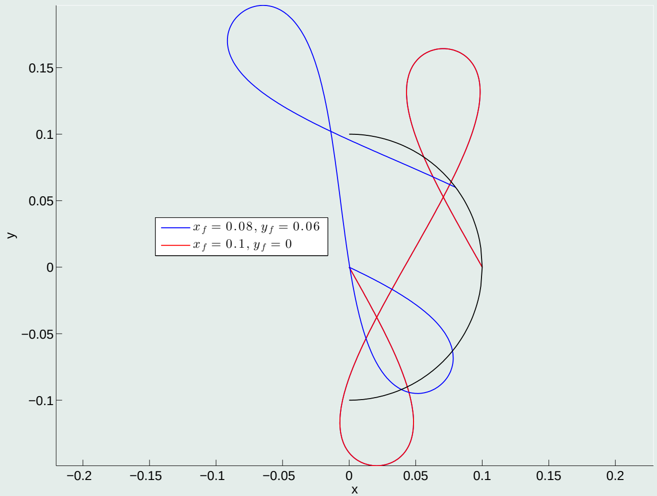
$\rightarrow$ need to set refined sufficient conditions (cf R. Vinter).

Circle as a right end-point constraint

$$\begin{cases} \dot{q} = \frac{\partial H}{\partial p}, \qquad \dot{p} = -\frac{\partial H}{\partial q}, \\ x(0) = 0, \quad y(0) = 0, \quad x(T)^2 + y(T)^2 - R^2 = 0, \\ \alpha_{1|2}(T) = \alpha_{1|2}(0), \quad \theta(T) = \theta(0), \\ p_{\alpha_{1|2}}(T) = p_{\alpha_{1|2}}(0), \quad p_\theta(T) = p_\theta(0), \\ p_x(T)y(T) - p_y(T)x(T) = 0. \end{cases}$$

Taking the initial position angle θ_0 as a parameter, minimizers are embed in a one-parameter family of minimizers.

$\rightarrow$ the non-uniqueness of minimizers.



Perspectives

- relations between the true system and its nilpotent approximation: continuation on small strokes of the nilpotent system.
- find other homotopy classes of strokes for the true system.
- existence of smooth abnormal strokes (difference with Copepod).
- refined second order sufficient conditions.

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