Geometric optimal control for microorganisms

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Life at low Reynolds number (Purcell, 1977)

\[ R = \frac{av \rho}{\eta} = \frac{av}{\nu} \]

\[ R \approx 10^2 \, \text{cm}^2 \text{sec}^{-1} \text{ for water} \]

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.

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

Dynamics.

\[ \dot{\theta} = H(\theta)\tau, \quad \tau = (x, y, \alpha). \]

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. \[ E(u) = \int_0^T (u H^{-1} u) dt. \]

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 \(D\).
\(D_1 = \text{span}\{F_1, F_2\}, \quad D_2 = D_1 \cup \text{span}\{[F_1, F_2]\}, \quad D_3 = D_2 \cup \text{span}\{[[F_1, F_2], F_1], [[F_1, F_2], F_2]\}. \)
At a point \(X_0\), \(D_1(X_0)\) is a \((2, 3, 5)\)–distribution.

- compute the nilpotent approximation 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 \((\theta_1, \theta_2)\) 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

$$\beta(t) = (\exp t F_2 \exp -t F_1 \exp -t F_2 \exp t F_1)(X(0))$$

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).

\[ x_0(t) = \frac{u_1 \sin(\theta_1) + u_2 \sin(\theta_2)}{2 + \sin^2(\theta_1) + \sin^2(\theta_2)}, \quad \dot{\theta}_1 = u_1, \quad \dot{\theta}_2 = u_2 \quad (\text{constraint: } 0 \leq \theta_1 \leq \theta_2 \leq \pi). \]

**Controlled dynamics.**

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

\[
M = \begin{pmatrix}
2 - 1/2(\cos^2(\theta_1) + \cos^2(\theta_2)) & -1/2 \sin(\theta_1) & -1/2 \sin(\theta_2) \\
-1/2 \sin(\theta_1) & 1/3 & 0 \\
-1/2 \sin(\theta_2) & 0 & 1/3
\end{pmatrix}
\]
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 $\pi$, while the unison sequence corresponds to a displacement from $\pi$ to 0 with the constraint $\theta_1 = \theta_2$. 
• The driftless control system is
\[ \dot{q}(t) = \sum_{i=1}^{2} u_i(t) F_i(q(t)) \]
where \( q = (x_0, \theta_1, \theta_2) \), \( F_i = \frac{\sin(\Delta)}{\Delta} \frac{\partial}{\partial x_0} + \frac{\partial}{\partial \theta_i} \) and \( \Delta = 2 + \sin^2(\theta_1) + \sin^2(\theta_2) \).

\[ \dot{z} = u_1 \vec{H}_1(z) + u_2 \vec{H}_2(z), \quad z = (q, p) \]
where \( \vec{H}_i \) are the Hamiltonian vector fields of the Hamiltonian lifts \( H_i(z) = \langle p, F_i(q) \rangle, i = 1, 2 \).

• Pontryagin Maximum Principle:
\[ \exists p(.) \in W^{1,1}([0, T]; \mathbb{R}^2) \text{ and a constant } p^0 \leq 0 \text{ such that for a.e. } t \in [0, T], \]
- \( (p(.), p^0) \neq (0, 0) \)
- \( \frac{\partial H}{\partial u} = 0 \) 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 $\pi$,

- $\theta_1 = \theta_2$.

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 $u_1 = u_2$.

**Remark.** A recent contribution proves that a trajectory with a corner of this type cannot be optimal.
Analysis outside the singular set $\Sigma$

\[ H_3 = \langle p, F_3(q) \rangle, \text{ with } F_3 = [F_1, F_2] \text{ and the set } \{ q, H_1, H_2, H_3 \} \text{ are coordinates.} \]

(the problem is isoperimetric since $p_1$ is a first integral: $\dot{p}_1 = 0$).

**Equations in the Poincaré coordinates.**

\[
\begin{align*}
\dot{H}_1 &= dH_1(\overrightarrow{H}_n) = \{H_1, H_2\} H_2 = H_2 H_3, \\
\dot{H}_2 &= dH_2(\overrightarrow{H}_n) = \{H_2, H_1\} H_1 = -H_1 H_3, \\
\dot{H}_3 &= dH_3(\overrightarrow{H}_n) = \{H_3, H_1\} H_1 + \{H_3, H_2\} H_2
\end{align*}
\]

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,

\[
\lambda_1 = \lambda_2 = 0, \quad \frac{\partial f}{\partial \theta_1} = \lambda_3 f \text{ and } \lambda'_1 = \lambda'_2 = 0, \quad \frac{\partial f}{\partial \theta_2} = \lambda'_3 f.
\]
We conclude that

\[ \dot{H}_1 = H_2 H_3, \quad \dot{H}_2 = -H_1 H_3, \]

\[ \dot{H}_3 = H_3 (\lambda_3 H_1 + \lambda'_3 H_2). \]

**Integration.** Time reparameterization: \( ds = H_3 dt \)

\[ \frac{dH_1}{ds} = H_2, \quad \frac{dH_2}{ds} = -H_1, \quad \frac{dH_3}{ds} = \lambda_3 H_1 + \lambda'_3 H_2. \]

Hence \( H_1'' + H_1 = 0 \) when differentiating with respect to the new time \( s \) (harmonic oscillator).
Furthermore with the approximation \( \lambda_3, \lambda'_3 \) 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:

\[
\begin{cases}
\dot{q} = \frac{\partial H_n}{\partial p}, & \dot{p} = -\frac{\partial H_n}{\partial q}, \\
x_0(0) = 0, & x_0(2\pi) = x_f, \\
\theta_1|2(0) = \theta_1|2(2\pi), & p_{2|3}(0) = p_{2|3}(2\pi).
\end{cases}
\]

where \(H_n\) is the true Hamiltonian in the normal case

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

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**.
**First conjugate time** $t_c$: the exponential map

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

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.
Comparisons of strokes

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

- $L(\gamma)$ is the length of the stroke $\gamma$ (*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 → related to count the number of strokes on each energy level.
- Micro swimmer devices with Takagi.
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 $x_0$, $D(x_0) = \text{span}\{F_1(x_0), \ldots, F_m(x_0)\}$.

- 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 \( \varphi \in \text{Diff}(M) \) acting on \( F_i \) such that:

\[
(\varphi \ast F_1)(x) = \hat{F}_1(x), \quad (\varphi \ast F_2)(x) = \hat{F}_2(x).
\]

\( \theta_1 = x_1 \) and \( \theta_2 = x_2 \) are invariant by the \( \varphi \).

**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 \((u, \text{sn}(u), \text{cn}(u), \text{dn}(u), E(u))\),

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

**Hamiltonian lifts.**

\[ H_1 = \langle p, \hat{F}_1(x) \rangle = p_1, \]
\[ H_3 = \langle p, [\hat{F}_1, \hat{F}_2](x) \rangle = -p_3 - 2x_1 p_5, \]
\[ H_5 = \langle p, [[\hat{F}_1, \hat{F}_2], \hat{F}_2](x) \rangle = p_4. \]

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

**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

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

\[ \dot{H}_2 = -H_3 H_1, \quad \dot{H}_3 = H_1 H_4 + H_2 H_5, \]
\[ \dot{H}_4 = 0 \quad \text{hence} \quad H_4 = c_4, \quad \dot{H}_5 = 0 \quad \text{hence} \quad H_5 = c_5. \]

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 \( \omega \) and \( \phi \) 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

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

where \( B \) is a constant.
Oscillating case. We set $u = \omega t + \phi_0$, $k$ is the modulus of elliptic functions.

$$x_1(u) = \frac{1}{\omega} \left[ x_1(\phi_0) - 2k \sin(\phi) \operatorname{cn}(u,k) + (-u + 2E(u,k)) \cos(\phi) \right],$$

$$x_2(u) = \frac{1}{\omega} \left[ x_2(\phi_0) - 2k \cos(\phi) \operatorname{cn}(u,k) + (u - 2E(u,k)) \sin(\phi) \right],$$

$$x_3(u) \ldots, x_4(u) \ldots, x_5(u) \ldots$$

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

![Family of eight shape strokes](image)
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.

\[ x_1(u) = (-2 \cos(\phi)u + 2 \cos(\phi) E(u/k,k) k - 2 \sin(\phi) \text{dn}(u/k,k) k + \cos(\phi) uk^2 + x_1(\phi_0) k^2) \omega^{-1} k^{-2}, \]
\[ x_2(u) = (2 \sin(\phi)u - 2 \sin(\phi) E(u/k,k) k - 2 \cos(\phi) \text{dn}(u/k,k) k - \sin(\phi) uk^2 + x_2(\phi_0) k^2) \omega^{-1} k^{-2}, \]
\[ x_3(u) \ldots x_4(u) \ldots x_5(u) \ldots \]

Family of strokes of **period** \(2\pi/\omega\).
Non self-intersecting and 8 solutions. There is no conjugate time $t_{1c} \in [0, 2\pi]$. 

Numerical simulations on the real system
Extremals with the same cost

Symmetry with respect to $\theta_0$.

**Lemma.** If $\theta(t), \alpha(t), \bar{x}(t), \bar{y}(t)$ is an extremal solution associated to $u(\cdot)$ 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 $u(\cdot)$ 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 $L^\infty$-topology
- this extremum is **locally unique**.

→ need to set refined sufficient conditions (cf R. Vinter).
Circle as a right end-point constraint

\[
\begin{aligned}
\dot{q} &= \frac{\partial H}{\partial p}, \\
\dot{p} &= -\frac{\partial H}{\partial q}, \\
x(0) &= 0, \\
y(0) &= 0, \\
x(T)^2 + y(T)^2 - R^2 &= 0, \\
\alpha_{1|2}(T) &= \alpha_{1|2}(0), \\
\theta(T) &= \theta(0), \\
p\alpha_{1|2}(T) &= p\alpha_{1|2}(0), \\
p\theta(T) &= p\theta(0), \\
p_x(T)y(T) - p_y(T)x(T) &= 0.
\end{aligned}
\]

Taking the initial position angle $\theta_0$ as a parameter, minimizers are embed in a one-parameter family of minimizers.

\[\rightarrow\] the non-uniqueness of minimizers.
• 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.

- Bonnard, B., Chyba, M., Rouot, J., Takagi, D.,: A Numerical Approach to the Optimal Control and Efficiency of the Copepod Swimmer (preprint)
