Taylor methods for computer assisted proofs

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The physical problem

The mathematical modelling of electric signalling in biological tissues, and in the cardiac muscle in particular, is a longstanding problem that has attracted a number of efforts. The mathematical structure of the differential models typically reads as a reaction–diffusion equation, linear in the diffusion and nonlinear in the reaction term, coupled with a one or more ordinary differential equations.

The physical problem

The classical model that preserves the basic mathematical nature of the problem while introducing the minimum amount of algebraic complications are the Fitzhugh–Nagumo equations:

$$\frac{\partial v}{\partial t} - \nabla \cdot (\mathbf{D} \nabla v) = -Av(v-\alpha)(v-1) - Aw \,,$$

$$\frac{\partial w}{\partial t} = v - \frac{w}{\tau} \,,$$

where $v(\mathbf{X}, t)$ is the action potential and $w(\mathbf{X}, t)$ is the gate variable. In general $\mathbf{D}$ is a symmetric positive definite tensor and $A \simeq ||D|| \gg 1$ where $||D||$ denotes some suitable norm.

The physical problem

Recent studies have pointed out the role of the contractility of the substratum in real physiological conditions, where the electrical potential actually modulates the contraction of the muscle fibers and then the strain of the material. The equations are therefore to be rewritten in moving coordinates, where the strain of the domain is driven by the action potential itself. It is convenient to rewrite the equations in material coordinates, using an mapping between current positions and reference ones. Adopting the standard terminology of continuum mechanics, we denote by $\mathbf{x} = \mathbf{x}(\mathbf{X}, t)$ the position at time t of the material point that was at time $t = 0$ in $\mathbf{X}$.

The physical problem

The gradient of deformation is therefore $\mathbf{F} = \frac{\partial \mathbf{x}}{\partial \mathbf{X}}$ and the equations read

$$\frac{\partial}{\partial t}(Jv) - \mathrm{Div}\,\left(J\mathbf{F}^{-1}\mathbf{D}\mathbf{F}^{-T}\mathrm{Grad}\,v\right) = -AJv(v-\alpha)(v-1) - AJw\,,$$

$$\frac{\partial}{\partial t}(Jw) = Jv - \frac{Jw}{\tau}\,,$$

where $J = \det(\mathbf{F})$. We are interested in the one dimensional version

$$\frac{\partial}{\partial t}(Jv) - \frac{\partial}{\partial X}D\left(J^{-1}\frac{\partial v}{\partial X}\right) = -AJv(v-\alpha)(v-1) - AJw\,,$$

$$\frac{\partial}{\partial t}(Jw) = Jv - \frac{Jw}{\tau}\,,$$

where the (scalar) diffusion coefficient D is taken constant and, simply, $J = \partial x/\partial X$.

The physical problem

To close the problem, we need to introduce a relation between the contraction of the substrate and the action potential. While this relation in real biological tissues involes quite complicated relations, we choose the simple linear relation

$$\frac{\partial x}{\partial X} = 1 - \beta v \,,$$

where β is a positive constant. We finally get

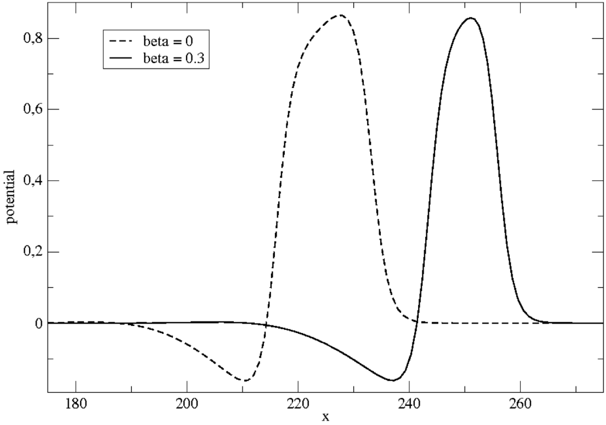
$$\varepsilon \frac{\partial}{\partial t}((1-\beta v)v) - D\frac{\partial}{\partial X}\left(\frac{1}{1-\beta v}\frac{\partial v}{\partial X}\right) = -(1-\beta v)v(v-\alpha)(v-1) - (1-\beta v)w \,,$$

$$\frac{\partial}{\partial t}((1-\beta v)w) = (1-\beta v)\left(v - \frac{w}{\tau}\right) \,.$$

where we have directly taken $A = D = \varepsilon^{-1}$.

Numerical results

In a past paper we have numerically found that the system above admits a travelling pulse solution that travels faster than in the rigid case.



Main result

Here we present a proof that such solution exist, together with a tight bound on its speed. Looking for solutions of travelling wave type and finite energy, amounts to looking for solutions $v(t,X) = V(X - ct)$, $w(t,X) = W(X - ct)$, where V and W are homoclinic to 0.
The system becomes

$$\begin{cases} \frac{V''}{1-\beta V} = & -\varepsilon c(1-2\beta V)V' - \frac{\beta (V')^2}{(1-\beta V)^2} \\ & +(1-\beta V)V(V-\alpha)(V-1) + (1-\beta V)W \\ W' = & \frac{W}{c\tau} - \frac{V}{c} - \frac{\beta}{c}V^2 \end{cases}$$

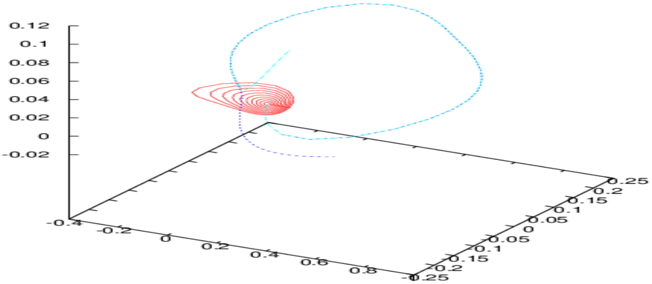
Theorem

Let $\alpha = 0.1$*,* $\beta = 0.3$*,* $\varepsilon = 0.01$*,* $\tau = 0.2$*. There exists* $c \in [\underline{c}, \bar{c}] = [59.173113678059, 59.173113678061]$ *such that the system above admits a solution homoclinic to* 0*.*

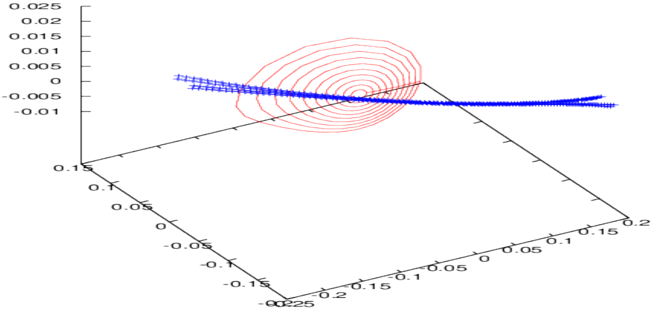
Proof

The strategy of the proof is based on following the unstable manifold until it comes back to the (local) stable manifold.

Problem: the intersection is not transversal. Numerically it looks as if the homoclinic solution exists only for a particular value of the parameter c.



Solution: solve the problem for all c and show that there must be an intersection.



Parameter dependence

A crucial step of the proofs consists in making all computations and estimates with a parameter that takes values in an interval. This issue one may define the parameter c as an interval with center c_0 and radius δ. But this approach is unfeasible in this proof: if one attempts to follow the unstable manifold using a parameter of finite width, however small, the errors accumulate very rapidly, and the computation gets quickly out of hand. Even a fine partition of the interval $[c_0 - \delta, c_0 + \delta]$ is not feasible.

Parameter dependence

Therefore, instead of an interval enclosure for c, we use a type `TBall`, which is a `Taylor` of order 2 with coefficients of type `Ball`. So every `Scalar` is effectively a function of c. We call ξ the parameter normalized to the interval $[-1, 1]$, so that c is represented by the `TBall`

$$\frac{\underline{c} + \bar{c}}{2} + \frac{\bar{c} - \underline{c}}{2}\xi\,.$$

By using `TBalls` as coefficients we obtain an explicit expression for a parametrization of the invariant manifolds, depending on both a geometrical parameter and c.

Invariant manifolds of dynamical systems

Consider the nonlinear dynamical system in $\mathbb{R}^N$

$$y' = Ay + B(y)\,, \tag{1}$$

with $A \in GL_N(\mathbb{R})$, $B : \mathbb{R}^N \to \mathbb{R}^N$ analytic, $B(0) = 0$, $\nabla B(0) = 0$. The unstable manifold is tangent in 0 to the eigenspace of A corresponding to eigenvalues with positive real part. The following theorem provides a mean of computing the unstable manifold in a neighborhood of the origin, in the case when A has pair of complex conjugate eigenvalues $\{\lambda, \bar{\lambda}\}$ with eigenvectors $\{v, \bar{v}\}$.

2-d invariant manifold

Theorem

Let $Z : \mathbb{C}^2 \to \mathbb{C}^N$ such that

$$Z(s_1, s_2) = \sum_{j,k=0}^{\infty} z_{jk} s_1^j s_2^k$$

converges when $|s_k| < 1$, $z_{jk} = 0$ if $j + k \leq 1$ and

$$\lambda s_1 Z_1(s_1, s_2) + \bar{\lambda} s_2 Z_2(s_1, s_2) = AZ(s_1, s_2) + B\big(s_1 v + s_2 \bar{v} + Z(s_1, s_2)\big), \quad (2)$$

where $Z_k = \frac{\partial Z}{\partial s_k}$. Then, for all $(r_1, r_2) \in \mathbb{C}^2$ such that $|r_k| < 1$ and all $t \leq 0$ the function

$$y(t) = r_1 e^{\lambda t} v + r_2 e^{\bar{\lambda} t} \bar{v} + Z\left(r_1 e^{\lambda t}, r_2 e^{\bar{\lambda} t}\right)$$

is a solution of equation (1). If additionally $r_2 = \bar{r}_1$, then $y(t) \in \mathbb{R}^N$.

2-d invariant manifold

Let $R > 0$, let $\mathcal{X}_R^2$ be the space of functions of two complex variables which can be written as a power series

$$Z(s_1, s_2) = \sum_{j,k=0}^{\infty} z_{jk} s_1^j s_2^k \tag{3}$$

with $z_{jk} \in \mathbb{C}^N$ and such that

$$\|Z\| := \sum_{j,k=0}^{\infty} |z_{jk}| R^{j+k}$$

converges. The space $\mathcal{X}_R^2$ is a Banach algebra.

2-d invariant manifold

In order to represent any function in $\mathcal{X}_R$ by using only a finite set of coefficients plus an estimate on the remainder. Our choice is to write functions as follows:

$$Z(s_1, s_2) = \sum_{j,k\geq 0}^{j+k\leq N} z_{jk} s_1^j s_2^k + E_Z\,, \tag{4}$$

where E_Z is a function in $\mathcal{X}_R^2$ with all coefficients of degree less or equal to N equal to zero.

Trasforming the problem into a fixed point problem

We write equation (2) as

$$z(s) = D_\lambda^{-1}(Az(s) + N(sv + z(s)))\,,$$

where D_λ^{-1} is defined by

$$D_\lambda^{-1}(s_1^j s_2^k) = \frac{s_1^j s_2^k}{j\lambda + k\bar{\lambda}}$$

Let $\mathcal{Z}_R$ be the subalgebra of the functions in $\mathcal{X}_R$ with zero constant and first degree term, and note that, if $z \in (\mathcal{Z}_R)^N$ and

$$\tilde{z}(s) = D_\lambda^{-1}(Az(s) + B(sv + z(s)))\,,$$

then $\tilde{z} \in (\mathcal{Z}_R)^N$, so we have defined an operator $C : (\mathcal{Z}_R)^N \to (\mathcal{Z}_R)^N$ by $\tilde{z} = C(z)$ and its fixed points correspond to the solution that we are looking for.

Finding the fixed point

We observe that, thanks to the compactness of C, it is feasible to build a Newton-like (local) contraction which is useful both for computing an approximated fixed point and for proving that there exists a (true) fixed point close to it.
Let $P : \mathcal{Z}_R^N \to \mathbb{C}^m$ be the map that returns the coefficients of the terms of order less than m. We define a matrix $M \in GL_m(\mathbb{C})$ as a finite dimensional approximation of $D(PCP) - I$, I being the identity map. Let $\mathcal{N} : \mathcal{Z}_R^N \to \mathcal{Z}_R^N$ be defined by

$$\mathcal{N}(Z) = C(Z) - M^{-1} * (C(Z) - Z)\,,$$

where for all $M \in GL_m(\mathbb{C})$ and all $Z \in \mathcal{Z}_R^N$ we define $M * z$ to be the function in $\mathcal{Z}_R^N$ with coefficients MPZ.

Finding the fixed point

A direct consequence of the contraction theorem is the following

Lemma

If there exist positive constants ε, r, K and $Z_0 \in \mathcal{Z}_R^N$ such that

- $\|\mathcal{N}(Z_0) - Z_0\| < \varepsilon$,
- $\|D\mathcal{N}(Z)\| \leq K$ *for all* $Z \in B_r(Z_0)$
- $\varepsilon + rK < 1$,

then there exists a unique fixed point of $\mathcal{N}$ (and therefore of C) in $B_r(Z_0)$.

And then we follow the unstable manifold

When we have a fixed point z of C, we have a rigorous enclosure of the unstable manifold tangent to v at 0, since such manifold intersects $sv + z(s)$ for all $s \in [0, R)$
Once we have good bounds on a point on the unstable manifold, away from the stationary point, we can follow the unstable manifold by solving

$$\begin{cases} y' & = Ay + N(y) \\ y(0) & = \bar{s}v + \bar{z}(\bar{s}) \, , \end{cases}$$

for some choice of $0 < \bar{s} < R$. To prove the existence of a homoclinic solution we need to prove that $y(t)$ belongs to the stable manifold of 0 as well.

Area-preserving maps

MacKay RG for pairs $P = (F, G)$ of area-preserving maps:

$$R(P) = (\widetilde{F}, \widetilde{G})\,, \quad \widetilde{F} = \Lambda^{-1} G \Lambda\,, \quad \widetilde{G} = \Lambda^{-1} F G \Lambda\,, \quad \Lambda = \begin{bmatrix} \lambda & 0 \\ 0 & \alpha \end{bmatrix}$$

Motivation: Observation of critical phenomena (self-similarity, universal scaling) during the breakup of invariant circles with rotation number

$$\vartheta^{-1} = \sqrt{5} - \frac{1}{2} = 0.618033988\ldots \qquad \text{(inverse golden mean)},$$

Area-preserving maps

In many families $\beta \mapsto G_\beta$, including the standard map

$$F_\beta(x,z) = (x-1,z)\,, \qquad G_\beta(x,z) = (x+w,w)\,, \quad w = z - \beta\sin(2\pi x)\,.$$

$\beta = 0$: smooth golden circle at $w = \vartheta^{-1}$.
$\beta > 0$ *small*: smooth golden circle persists, by KAM theory.

$\beta = \beta_*$: golden circle turns non-smooth and breaks up.

In suitable coordinates, the golden circle and nearby orbits are asymptotically invariant under a scaling $\Lambda = \begin{bmatrix}\lambda_* & 0\\ 0 & \alpha_*\end{bmatrix}$,

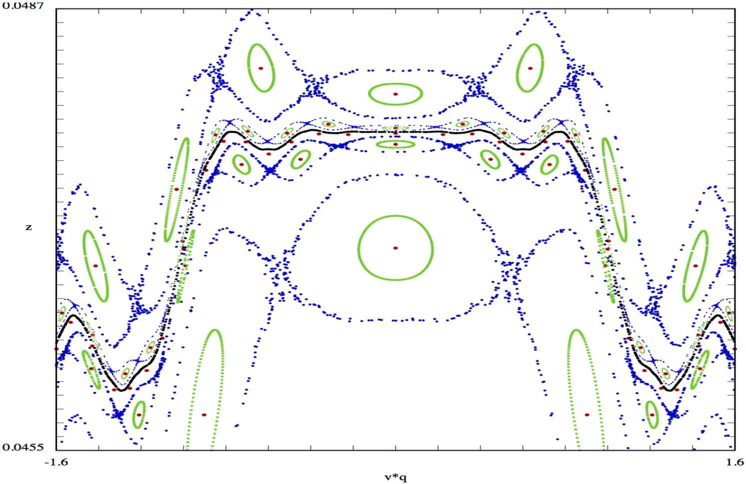
$$\lambda_* = -0.7067956691\ldots\,, \qquad \alpha_* = -0.3260633966\ldots\,,$$

with λ_* and μ_* universal (independent of the family).
This could be explained if

$$R^n(P_{\beta_*}) \to P_*\,, \qquad R(P_*) = P_*\,.$$

Critical area-preserving maps

Orbits for a **critical Hamiltonian**, [J. Abad, H.K., P. Wittwer:98]



Renormalization of area-preserving map

Find a pair $P = (F, G)$ of commuting area-preserving maps that is a fixed point of R,

$$R(P) = (\widetilde{F}, \widetilde{G}), \quad \widetilde{F} = \Lambda^{-1} G \Lambda, \quad \widetilde{G} = \Lambda^{-1} F G \Lambda, \quad \Lambda = \begin{bmatrix} \lambda & 0 \\ 0 & \alpha \end{bmatrix}$$

where λ and α are determined by the normalization condition $\widetilde{G}(0,0) = (-1, -1)$.

Renormalization of area-preserving map

Preserved but hard to deal with: **commuting** property $GF = FG$.
Desirable but not preserved: **reversibility** $G = SG^{-1}S$, with $S(x,z) = (-x,z)$.

Typical for computer-assisted proofs: first find appropriate reformulation.

Renormalization of area-preserving map

First reformulation: consider the transformation

$$N(G) = \Lambda^{-2} G F G \Lambda^2 \,, \qquad F = \Lambda^{-1} G \Lambda \,,$$

on a space of reversible maps G (preserved by N). Let $J = G^{-1}\Lambda^{-1} F G \Lambda$.
Lemma *If G is an analytic reversible fixed point of N, with the property that $|\lambda|^3 < |\mu| < |\lambda|^4$, and that $J \neq -\mathrm{Id}$, then $P = (F, G)$ is a fixed point of R and commuting.*

Renormalization of area-preserving map

Second reformulation uses generating functions: $G = \Gamma g$, where

$$G(x,z) = (y,w)\,, \qquad z = -\partial_x g(x,y)\,, \qquad w = \partial_y g(x,y)\,,$$

This defines a transformation $\mathcal{N} = \Gamma^{-1} N \, \Gamma$ for generating functions.

Third reformulation: contraction $\mathcal{M}(\phi) = \phi + \mathcal{N}(g_0 + M\phi) - (g_0 + M\phi)$.

Main result: existence of the critical fixed point

Theorem (G. A., H. Koch:09)

R has a fixed point $P_* = (F_*, G_*)$. The maps F_* and G_* are analytic, area-preserving, reversible, and they commute. The associated scaling Λ_* satisfies $\lambda_* = -0.7067956691\ldots$ and $\alpha_* = -0.3260633966\ldots$.

(Earlier partial results by [A. Stirnemann:97])

Implementation details

The computer uses `Taylor` series in two "variables" **u** and **v**,

$$g = \sum_{m,n} a_{m,n}\mathbf{u}^m\mathbf{v}^n + \mathbf{t}\sum_{m,n} b_{m,n}\mathbf{u}^m\mathbf{v}^n\,,$$

($b_{m,n} = 0$ if g is the generating function of a reversible map), where

$$\mathbf{u} = \left[\, t^2 - t_0^2 \,\right] + cv\,, \qquad \mathbf{v} = \mathbf{s} - s_0\,,$$

and

$$\mathbf{t}(x,y) = x + y\,, \qquad \mathbf{s}(x,y) = x - y\,,$$

with $t_0 = 51/128$, $s_0 = 307/256$, and $c = 3$.