First CET presentation

Kyunghoon HAN

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Outline

1. Introducing myself & the QUIRE project
2. Courses taken in 2021-2022 & why
3. Works
4. Possible research direction
5. Q & A

Educational background

Master of Science at the Université de Tours

- **Major** : Nonlinear theoretical physics
- **Research project** : Simulation of vortex behaviour in the inner-crust of a neutron star

Bachelor of Mathematics at the University of Waterloo

- **Major 1** : Pure Mathematics
- **Major 2** : Mathematical Physics
- **Physics research project** : On osmotic compaction of bacterial chromosomes

Scientific professional career

Career

- **SRuniverse, Seoul** Text-to-speech/speech-to-text, AI-generated YouTube celebrity, chat-bot, etc.
- **Hankook Life Science Institute, Seoul** Post-mortem physical cause-of-death analysis on mammals (mostly on rodents)
- **Canada Centre for Remote Sensing, Ottawa** Satellite image correction/analysis, satellite orbit inter/extrapolation, etc.

Research papers

- Kyunghoon Han, *On a stochastic construction of kinematics in discrete space-time*. Canadian Journal of Physics **93**, 5 (2015). `https://doi.org/10.1139/cjp-2014-0360`
- Nat Commun **13**, 3387 (2022) – to be reintroduced later in the slides

The QUIRE project

'Infra red (IR) spectra are the canary which does not sing if Angstrom-scale molecular dynamics are not correct'

from the project proposal

Improved prediction of IR spectra

- re-organize the view of dynamics as **structures in phase space**
- better algorithm to predict the IR spectra from the force-fields

Tools: chaos theory, hydrodynamics, polymer physics, etc.

Courses taken in 2021-2022

List of courses taken

In total, earned $10 + 1$ ECTS credits out of the required 20 credits in the past year.

Courses offered by the Department of Physics and Materials Science:

- "Group theory for condensed matter physics"
- "Structural and chemical characterisation of materials"

Courses offered by the Department of Mathematics:

- "Large deviations and asymptotics of diffusion processes"
- "Stochastic analysis on manifolds"

Motivation behind the large deviations theory

Example from physics

Consider an overdamped physical particle in a potential landscape provided by a weakly periodic potential $\tilde{U}(t,x)$ for $t \geq 0$ and $x \in \mathbb{R}^d$ with $\tilde{U}(kT+t,\cdot) = \tilde{U}(t,\cdot)$ for a **very large** period T.
If the system is under an influence of some white noise with intensity ϵ, the motion of the particle is given by the following stochastic differential equation (SDE):

$$dY^{\epsilon}(t) = -\nabla \tilde{U}\left(t, Y^{\epsilon}(t)\right) dt + \sqrt{\epsilon} dW(t)$$

One can rewrite the above SDE so that the period is 1, i.e. $t \mapsto t/T$, $U(t,x) = \tilde{U}\left(t/T, x\right)$, $t \geq 0$, $x \in \mathbb{R}^d$, then

$$dX^{\epsilon}(t) = -\nabla U\left(t, X^{\epsilon}(t)\right) dt + \sqrt{\epsilon} dW(t)$$

Questions one can ask from the example above

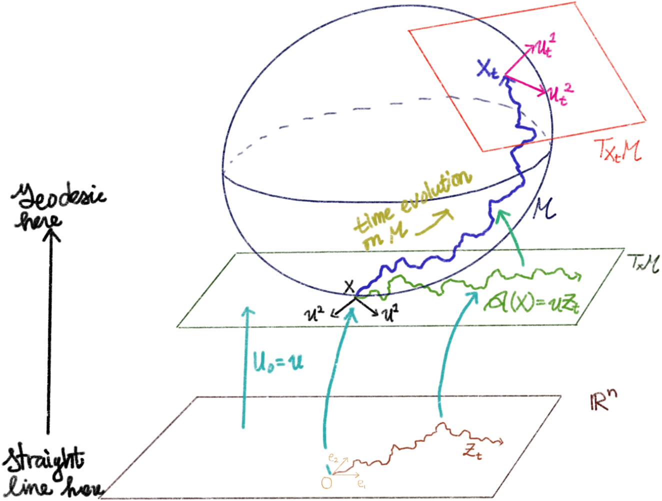
- What is the period of the oscillation in a given time interval?
- When would the oscillation terminate?
- What is the final state of the particle of interest?
- What happens if $T \to \infty$?

These questions are essentially connected to the asymptotic behaviours and the stochastic processes induced by the particle of interest.

Other examples found in physics

- Langevin dynamics $M\ddot{X} = \nabla U(X) - \gamma \dot{X} + \sqrt{2\gamma k_B T}\dot{W}(t)$
- Milankovitch cycles $c\frac{dT(t)}{dt} = Q(t)(1 - a(T(t))) - \sigma T(t)^4 + \sqrt{\epsilon}\dot{W}$
- Long-term climate changes
- Long term chemical reactions & change in conformations

Why is stochastic Riemannian geometry useful?



Relevance to physics - heat equation on curved space

Criteria on satisfying the heat equation

If a global section f of the vector bundle E is given, and $\tau_t f(X_t)$ is an E_{X_0}-valued process. Making $u(t,x) = E_x\left[\tau_t f(X_t)\right]$ a global section of E. Then, there exists a **horizontal Laplacian**, Δ^H such that

$$\frac{\partial u}{\partial t} = \frac{1}{2}\Delta^H u.$$

Normally, $\Delta^H f = g^{jk}\nabla_j\nabla_k f - g^{jk}\Gamma^i{}_{jk}\nabla_i f$, but with appropriate basis $(e_i)_i$,

$$\Delta^H f = \sum_{i=1}^{n} \nabla^2 f(e_i, e_i).$$

Noting that Δ is a second-order elliptic operator where $\Delta - \Delta^H$ is a linear transformation on each fibre; making the problem more solvable.

Works

Molecular graphics

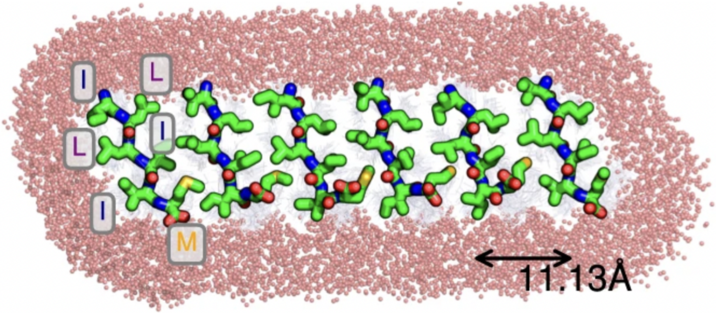


Figure: The figure I drew for the publication: Charnley, M., Islam, S., Bindra, G.K., Guneet K. Bindra, Jeremy Engwirda, Julian Ratcliffe, Jiantao Zhou, Raffaele Mezzenga, Mark D. Hulett, **Kyunghoon Han**, Joshoua T. Berryman, Nicholas P. Reynolds, *Neurotoxic amyloidogenic peptides in the proteome of SARS-COV2: potential implications for neurological symptoms in COVID-19*. Nat Commun **13**, 3387 (2022). `https://doi.org/10.1038/s41467-022-30932-1`

Peak detection for an input signal

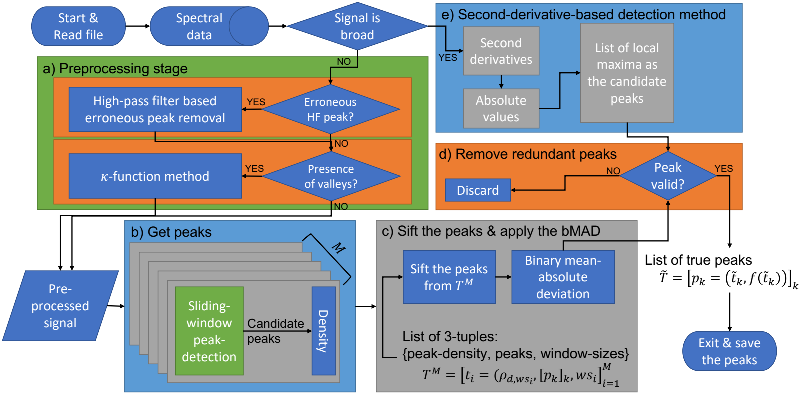
Motivation

Development of peak-detection algorithm that is free and easy-to-use for all.

Peak detection algorithms are useful for

- financial market data analysis
- radar signal interpretations
- acoustic chirp-signal identifications
- NMR, X-ray and IR spectral data analysis

Workflow of the algorithm



Definition of a peak

Definition (A peak with threshold)

For a connected and compact domain $\mathcal{D}$, let $\varphi : \mathcal{D} \to \mathbb{R}$ be a smooth and bounded function. The **peak** of the function φ with ϵ-threshold on $\mathcal{D}$, $p_\epsilon^{\mathcal{D}}$, is a map defined as:

$$f \mapsto p_\epsilon^{\mathcal{D}} = \begin{cases} (x^*, f(x^*)) & \text{if } \sup_{x \in \mathcal{D}} f(x) - \inf_{x \in \mathcal{D}} f(x) \geq \epsilon \\ 0 & \text{otherwise} \end{cases}$$

where $x^* = \arg\max_{x \in \mathcal{D}}(f)$ and $\epsilon > 0$.

Multi-window peak-detection - definition of a window

Definition (Sliding window)

Let $\mathcal{D} = [a, b] \subset \mathbb{R}$ be an interval with $a < b$. Define a window $\mathbf{w}^0$ of size ℓ in $\mathcal{D}$ where ${\mathbf{w}^0}_1 = a$, ${\mathbf{w}^0}_\ell = c \in \mathcal{D}$. Define the window **slid by a hop-size** h of $\mathbf{w}^0$ by

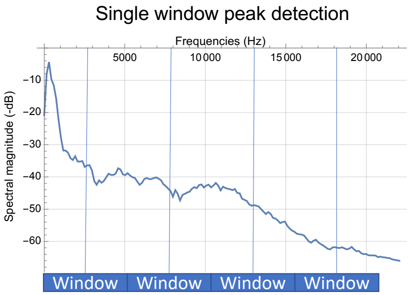
$$\mathbf{w}^1 = [a + h, c + h].$$

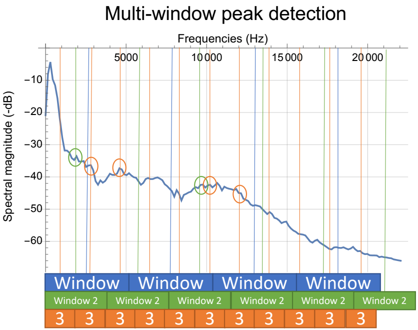
and the **sliding windows covering** $\mathcal{D}$ is a set of windows

$$\left\{ \mathbf{w}^i = [a + ih, c + ih] \middle| \, i = 0, \ldots, k \text{ such that } c + kh = b \right\}. \tag{1}$$

Multi-window peak-detection

Periodogram of an audio file recording done by the author





Discrimination of false peaks - bMAD, definitions 1

Definition (Median absolute deviation (MAD))

$MAD(X) = \frac{|X - \mathrm{med}(X)|}{\mathrm{med}(X - \mathrm{med}(X))}$

Definition (Selector function)

Let $\theta > 0$, then the selector function is defined as

$$S(x, \theta) = \begin{cases} 1 & \text{if } x > \theta \\ 0 & \text{otherwise} \end{cases}$$

for $x \in \mathbb{R}$.

Discrimination of false peaks - bMAD, definitions 2

Definition (Circular structural element)

A circular structural element of length i is defined as

$$E_i = \left(0, \cdots, 0, \underbrace{1, 0, \cdots, 0, 1}_{i}, 0, \cdots, 0 \right). \tag{2}$$

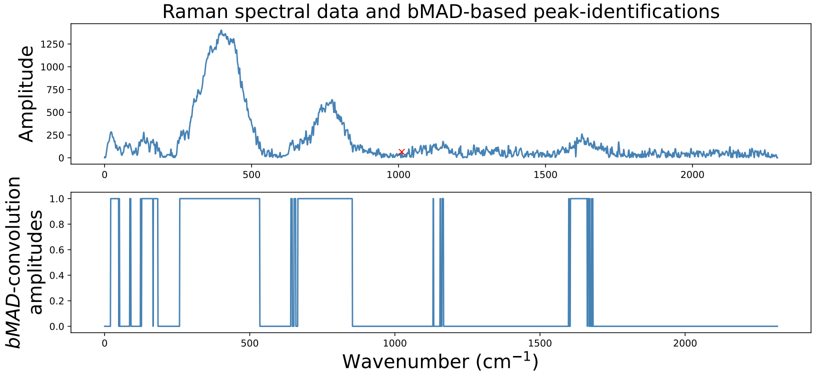
Definition (Binary MAD (bMAD))

$$bMAD(X) = (bMAD_1(X), \cdots, bMAD_N(X)) \tag{3}$$

$$bMAD_i(X) = S\left(MAD\left(E_i \star X\right), \theta\right) \tag{4}$$

where E_is are structural element vectors with length i.

Effectiveness of bMAD



bMAD Theorem

Theorem (Profile of *bMAD* on a peak)

Let φ be a continuous distribution with finite number of peaks. One can then find a value of the selector threshold θ so that bMAD(φ) as described in the Equation (3) with circular structural elements has 1s only in the domain where the peaks are.

The proof of this theorem is written in the manuscript I prepared for the submission... essentially the existence of $\theta > 0$ was proven using contradiction.

IR signal decomposition - idea

Treat an input broad signal as a sum of known distributions.

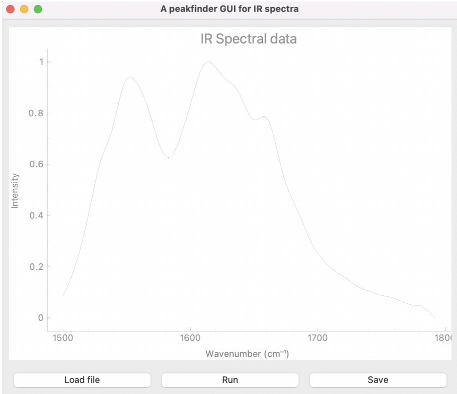
Problem

The decomposition is not unique.

Another problem

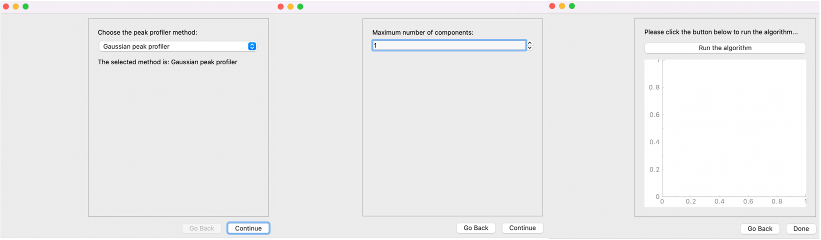
The non-uniqueness still confuses me

IR signal decomposition - main GUI page

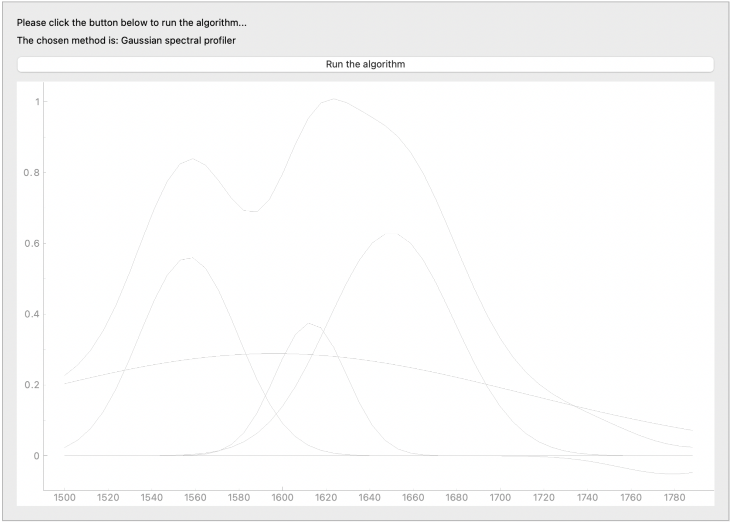


Data credit: Dr. Francesco Simone Ruggeri of the Department of Agrotechnology and Food Sciences, University of Wageningen

IR signal decomposition - wizard pages

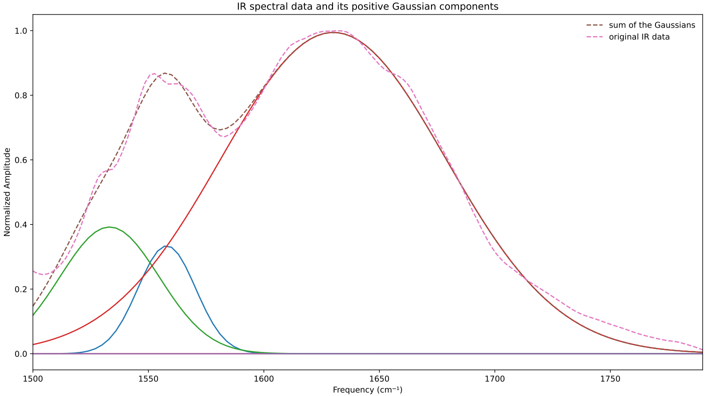


IR signal decomposition - result



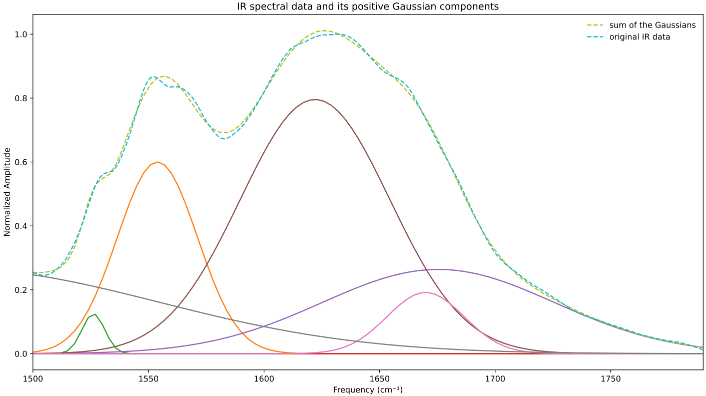
Gaussian decomposition of the signal - max 5 components

With at most 5 decompositions,

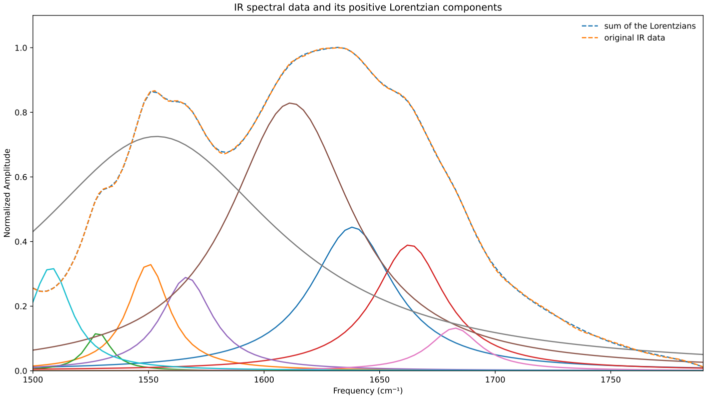


Gaussian decomposition of the signal - max 8 components

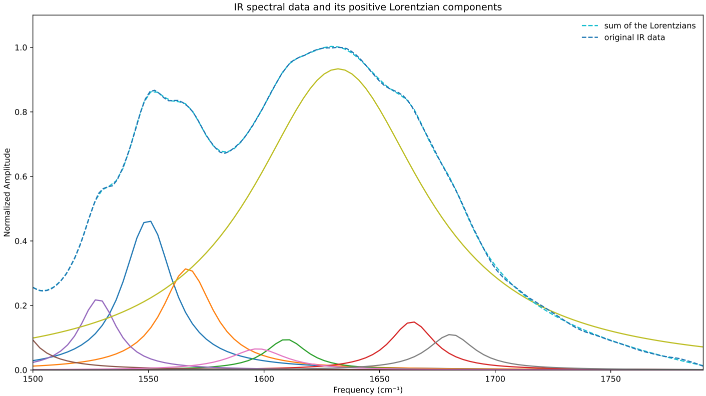
With at most 8 decompositions,



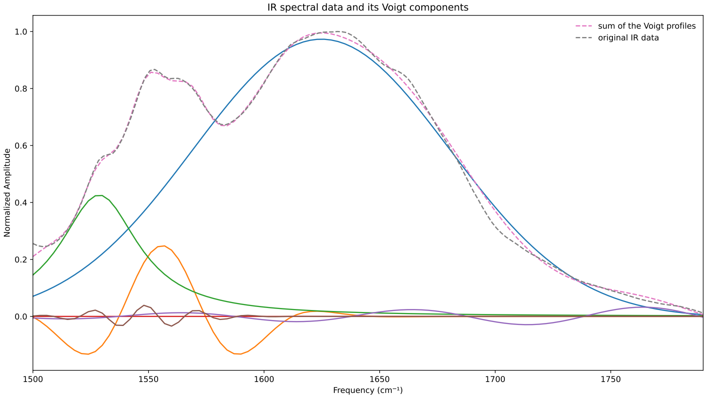
Lorentzian decomposition of the signal - without bounds



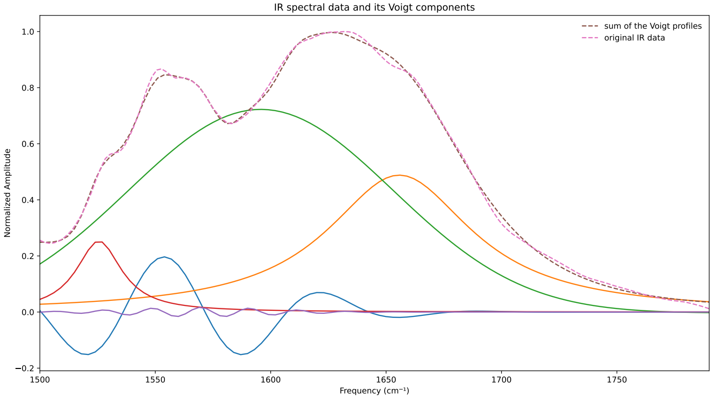
Lorentzian decomposition of the signal - max 8 components



Voigt decomposition of the signal - max 6 components



Voigt decomposition of the signal - max 5 components



Possible research direction

IR-spectral data prediction

Experimental challenges

- peak shifts
- peak broadening
- entirely new peaks
- thermal expansion anomalies

Current standard theoretical approaches

- diagonalisation of the Hessian for phonon spectra
- autocorrelation functions in dipole moment from a long MD simulations & consequent acquisition of IR spectra from its Fourier transformation

Classical force fields and its innate chaos

Example: Double nonlinear resonances in diatomic molecules

Given the reduced mass, $\mu = \frac{m_1 m_2}{m_1 + m_2}$, angular momentum, $\ell^2 = \ell_\theta^2 + \frac{\ell_\varphi^2}{\sin^2\theta}$, and the central potential, $U(r)$, the Hamiltonian is given as:

$$H = \frac{\mu \dot{r}^2}{2} + \frac{\ell^2}{2\mu r^2} + U(r).$$

G. V. López, A. P. Mercado *Journal of Modern Physics*, **6**,4 (2015), DOI:10.4236/jmp.2015.64054

Example continued: chaos due to the external electric field

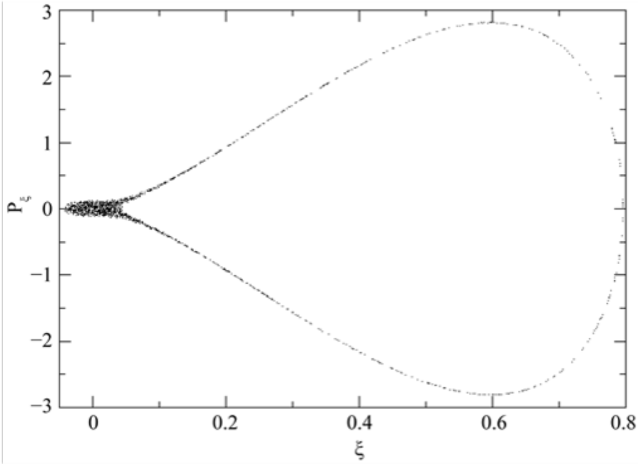
With the introduction of some external electric field, the problem reduces to solving the following system of equations:

$$\begin{aligned}
\dot{\xi} &= \frac{P_\xi}{2\mu} \\
\dot{P}_\xi &= qE_0 \cos(\varphi - \omega t) - \mu\omega_0^2 \xi + 3a^3 D\xi^2 \\
&\quad - \frac{7}{3} a^4 D\xi^3 - \frac{\ell^2}{2\mu r_0^2}\left(-\frac{2}{r_0} + \frac{6\xi}{r_0^2} - \frac{12\xi^2}{r_0^3} + \frac{20\xi^3}{r_0^4}\right) \\
\dot{\varphi} &= \frac{P_\varphi}{\mu r_0^2}\left(1 - \frac{2\xi}{r_0} + \frac{3\xi^2}{r_0^2} - \frac{4\xi^3}{r_0^3} + \frac{5\xi^4}{r_0^4}\right) \\
\dot{P}_\varphi &= -qE_0 \xi \sin(\varphi - \omega t)
\end{aligned}$$

Question

For what value of E_0 is the system chaotic?

Poincaré map of the example



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Construction of periodic orbits of high-dimensional chaotic systems

Given a autonomous PDE of the form $f(\vec{u}) - \vec{u} = \vec{0}$, one can write its governing equation as

$$-\frac{1}{T}\frac{\partial \vec{u}}{\partial s} + \mathbf{N}(\vec{u}) = \vec{0}$$

Loop

A loop $\mathbf{l}(\vec{x}, s)$ is a tuple of a field $\vec{u}(\vec{x}, s)$ and a period T.

Sajjad Azimi, Omid Ashtari, and Tobias M. Schneider *Physical Review E* **105**, 014217

Some of the authors' definitions

Definition (Loop space)

Where $\vec{u}$ satisfies the BC at $\partial\Omega$ and is periodic in s, the loop space is defined as:

$$\mathcal{P} = \left\{ \mathbf{l}\,(\vec{x}, s) = \begin{pmatrix} \vec{u}(\vec{x}, s) \\ T \end{pmatrix} : \vec{u} : \Omega \times [0, 1)_{\text{periodic}} \to \mathbb{R}^n, T \in \mathbb{R} \right\}$$

Definition (Generalized loop space)

If $\vec{q}_1$ is periodic in s, the generalized loop space is defined as:

$$\mathcal{P}_g = \left\{ \mathbf{q}\,(\vec{x}, s) = \begin{pmatrix} \vec{q}_1(\vec{x}, s) \\ q_2 \end{pmatrix} : \vec{q}_1 : \Omega \times [0, 1)_{\text{periodic}} \to \mathbb{R}^n, q_2 \in \mathbb{R} \right\}$$

Note that the generalized loop space does not require the BCs to be satisfied in the spatial domain and clearly $\mathcal{P} \subset \mathcal{P}_g$.

Evolve the cost function

Recipe

- define the initial loop : $\mathbf{l}_0 \in \mathcal{P}$
- reparametrize the time as: $\mathbf{l}(\tau) = \begin{pmatrix} \vec{u}\,(\vec{x}, s; \tau) \\ T(\tau) \end{pmatrix}$
- define a new evolution equation as: $\frac{\partial \mathbf{l}}{\partial \tau} = G(\mathbf{l})$.

The operator G is chosen so that $\frac{\partial J}{\partial \tau} \leq 0$ for all fictitious time τ.

Physicality of the cost-function

The goal is to quantify how far is the chosen loop from the stable orbit in the phase-space. The cost-function quantifies the scalar distance between two functionals: $\mathbf{l}(\tau)$ and the physically valid trajectory.

Thank you for your attention.