A Computer-assisted proof for a steady state of a chemotaxis model

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Let $l \in \mathbb{R}_+$, $\sigma \geq 0$ the logistic parameter, $d > 0$ the diffusion rate, and γ the motility function, positive and decreasing.

PDE of Keller-Segel type: cross-diffusion and logistic reaction, [KS71; WX21].

$$\begin{cases} \partial_t u = \Delta(\gamma(v)u) \quad + \sigma u(1-u), & (x,t) \in (0,l) \times \mathbb{R}_+^* \\ \partial_t v = d\Delta v \quad + u - v, & (x,t) \in (0,l) \times \mathbb{R}_+^* \\ \partial_x u(x,t) = 0, \quad \partial_x v(x,t) = 0, & (x,t) \in \{0,l\} \times \mathbb{R}_+^* \end{cases} \tag{1}$$

Where u and v represent cells concentration and chemical concentration, respectively.

Study of the stationary states to understand the longtime behavior of solutions of the 'K-S equation' (1).

Stationary equation

$$\begin{cases} \Delta(\gamma(v)u) + \quad \sigma u(1-u) = 0, & x \in (0,l) \\ d\Delta v + \quad u - v = 0, & x \in (0,l) \\ \partial_x u(x) = 0, \quad \partial_x v(x) = 0, & x \in \{0,l\} \end{cases} \tag{2}$$

Remark: For all σ, $(1,1)$ is a solution of (2).

We can look for solutions of the stationary problem (2) on the form:

$$u(x) = u_0 + 2\sum_{k=1}^{+\infty} u_k \cos\left(\frac{k\pi}{l}x\right) \text{ and } v(x) = v_0 + 2\sum_{k=1}^{+\infty} v_k \cos\left(\frac{k\pi}{l}x\right).$$

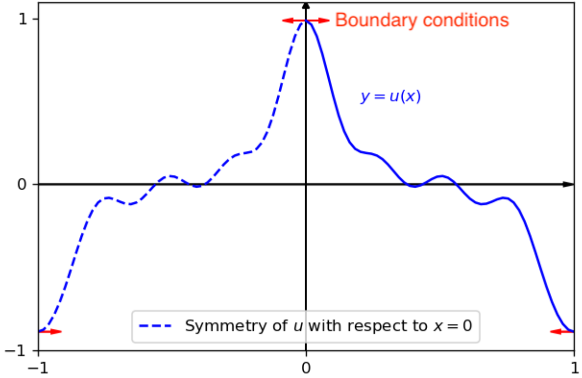

Figure: Geometric justification

The model

Let $\mathbf{u} = (u_0, u_1, \ldots, u_k, \ldots) = (\mathcal{F}_k(u))_{k\in\mathbb{N}}$, $\mathbf{v} = (\mathcal{F}_k(v))_{k\in\mathbb{N}}$ and $\gamma(\mathbf{v}) = (\mathcal{F}_k(\gamma \circ v))_{k\in\mathbb{N}}$.

With the discrete convolution and the Laplacian in $1D$, $\Delta = \text{diag}\left(0, -(\frac{\pi}{l})^2, -(\frac{2\pi}{l})^2, \ldots, -(\frac{k\pi}{l})^2, \ldots\right)$, we have:

Fourier Sequences Equation

$$\begin{cases} \Delta\left(\gamma(\mathbf{v}) * \mathbf{u}\right) & + \quad \sigma\mathbf{u} * (\mathbf{1} - \mathbf{u}) & = \mathbf{0} \\ d\Delta\mathbf{v} & + \quad \mathbf{u} - \mathbf{v} & = \mathbf{0} \end{cases} \tag{3}$$

It can be written as follows $F(\mathbf{u}, \mathbf{v}) = (\mathbf{0}, \mathbf{0})$.

We apply the well-known Newton's Method !

Firstly, we calculate item-by-item the derivative of F in $\mathbf{U} = (\mathbf{u}, \mathbf{v})$:

$$DF(\mathbf{u}, \mathbf{v}) = \begin{pmatrix} \Delta\gamma(\mathbf{v}) + \sigma(\mathbf{1} - 2\mathbf{u}) & \Delta\gamma'(\mathbf{v}) * \mathbf{u} \\ \mathbf{1} & d\Delta - \mathbf{1} \end{pmatrix}. \tag{4}$$

Fast method: With $\mathbf{U} = (\mathbf{u}, \mathbf{v})$, $\mathbf{U}_{k+1} = \mathbf{U}_k - [DF(\mathbf{U}_k)]^{-1} F(\mathbf{U}_k)$ with $\mathbf{U}_0$ a **perturbation** of $(\mathbf{1}, \mathbf{1})$. We call $\mathbf{U}_{final}$ the last iteration we choose.

Theorem on the instability of the trivial state

Assume we have the following conditions satisfied

$$\begin{cases} (\gamma(1)+\gamma'(1)+d\sigma)^2 - 4d\sigma\gamma(1) & \geq & 0 \\ \gamma(1)+\gamma'(1)+d\sigma & < & 0 \end{cases} \tag{5}$$

Then the stationary state $(\mathbf{1}, \mathbf{1})$ is *unstable*. And we know the direction (in ℓ^1_ν) of instability.
Otherwise, it is *linearly stable*.

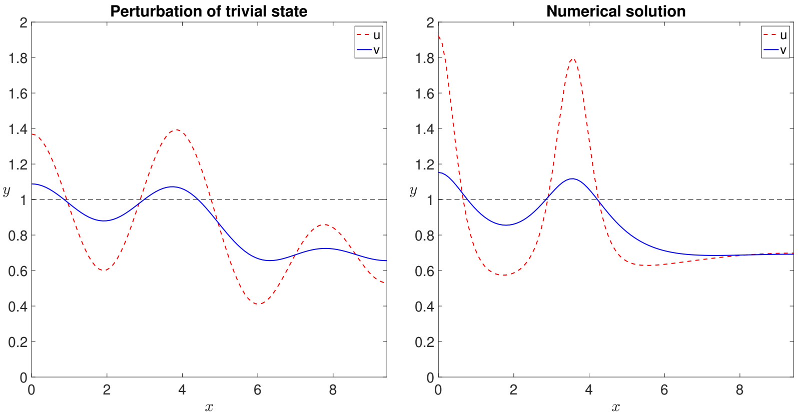

Figure 2: $\sigma = 0.053$, $\gamma(x) = \dfrac{1}{1+x^9}$, $d = 1$, and $l = 3\pi$

Approximate solutions

II) A good guess. From [WX21].

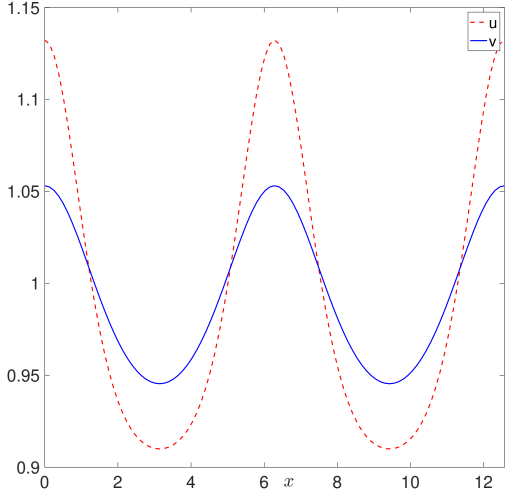

Figure 3: $\sigma = 0.6$, $\gamma(x) = \dfrac{1}{1+\exp(9(x-1))}$, $d = 1$, and $l = 4\pi$

To calculate, we see our sequences in the Banach algebra ℓ^1_ν which is the set that contains the sequences $\mathbf{u}$ such that :

$$\|\mathbf{u}\|_\nu := |u_0| + 2\sum_{k=1}^{+\infty} |u_k|\nu^k \; < +\infty, \; \nu \geq 1.$$

We compute $F(\mathbf{u}, \mathbf{v}) \in (\ell^1_\nu)^2$, and $DF(\mathbf{u}, \mathbf{v}) \in \mathcal{L}((\ell^1_\nu)^2)$.

BUT ...

Reminder: $(\ell^1_\nu, *, \|\cdot\|_\nu)$ is a Banach algebra means, $(\ell^1_\nu, \|\cdot\|_\nu)$ is a complete normed space and $(\ell^1_\nu, *, +)$ is an associative algebra, with $*$ satisfying $\|\mathbf{u} * \mathbf{v}\|_\nu \leq \|\mathbf{u}\|_\nu \|\mathbf{v}\|_\nu$. The identity element is $\mathbf{1}$.

I do not know how to literally inverse this operator ...
In other words, the calculation of $[DF(\mathbf{U})]^{-1}$ in the " Newton's method" earlier is rigorously false.

To overcome this obstacle we use a fixed-point method adapted from the Newton's one on the functional $\mathbf{U} \mapsto \mathbf{U} - AF(\mathbf{U})$ with A an **approximate inverse** of $DF(\overline{\mathbf{U}})$ in $\mathcal{L}((\ell^1_\nu)^2)$, $\overline{\mathbf{U}}$ a **finite approximate solution**.

With A well-chosen, injective, numerically calculable and satisfying the following assertions.

Newton-Kantorovitch Theorem

Let $\nu > 1$, assume there exist Y, Z_1, Z_2 and $r^* > 0$ satisfying :

$$\|AF(\overline{\mathbf{U}})\|_\nu \leq Y \tag{6a}$$
$$\|I - ADF(\overline{\mathbf{U}})\|_\nu \leq Z_1 \tag{6b}$$
$$\|AD^2F(\mathbf{U})\|_\nu \leq Z_2, \quad \forall \mathbf{U} \in \mathcal{B}(\overline{\mathbf{U}}, r^*) \tag{6c}$$

$$Z_1 < 1 \tag{7a}$$
$$2YZ_2 < (1 - Z_1)^2 \tag{7b}$$

Then for all r such that

$$\frac{1 - Z_1 - \sqrt{(1 - Z_1)^2 - 2YZ_2}}{Z_2} \leq r < \min(r^*, \frac{1 - Z_1}{Z_2})\,, \tag{8}$$

There exist a unique solution $\mathbf{U}^* \in \mathcal{B}_\nu(\overline{\mathbf{U}}, r)$ of the ‘Fourier equation’ (3). The functions (u^*, v^*) described by the Fourier sequences $(\mathbf{u}^*, \mathbf{v}^*)$ are solutions of the stationary problem (2).

Approximated inverse of the differential

According to [Bre22], we choose

$$A = \left(\begin{array}{c|c} \boxed{A^{11}} \quad \mathbf{w}^{11}\Delta^{-1} & \boxed{A^{12}} \quad \mathbf{w}^{12}\Delta^{-1} \\ \hline \boxed{A^{21}} \quad \mathbf{w}^{21}\Delta^{-1} & \boxed{A^{22}} \quad \mathbf{w}^{22}\Delta^{-1} \end{array}\right), \tag{9}$$

with

$$\left(\begin{array}{c|c} \mathbf{w}^{11} & \mathbf{w}^{12} \\ \hline \mathbf{w}^{21} & \mathbf{w}^{22} \end{array}\right), \text{ the inverse of } \begin{pmatrix} \gamma(\bar{v}) & \gamma'(\bar{v})\bar{u} \\ 0 & d \end{pmatrix} \text{ in } \ell^1_\nu$$

and A^{ij} are from the inverse of a finite dimensional projection of $DF(\bar{\mathbf{u}}, \bar{\mathbf{v}})$.

Here, the choice of A is balanced between **what can be known by approximation** (the information given by the computer) and **what must be known by estimation** (the information provided by the mathematician).

In the literature [Des+19; Bre22; MPW20; WX21], we are interested in several types of γ : polynomial, power series, rational fraction. We want to manage all these cases. In order to obtain the inequalities of the 'N-K Theorem' (5) we need to answer the following questions:

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- Given an analytical expression of γ, can we find a "good" approximation of $\gamma(\bar{\mathbf{v}})$, called $\underline{\gamma(\bar{\mathbf{v}})}$, in ℓ^1_ν for any $\bar{\mathbf{v}}$ finite?

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⋆ Taylor Expansion

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Two ideas :

- ⋆ Taylor Expansion
- ⋆ Neumann series

Let $\mathbf{x}, \mathbf{y} \in \ell^1_\nu$. Assume we have $\underline{\mathbf{x}}$ and $\underline{\mathbf{y}}$ approximations of $\mathbf{x}$ and $\mathbf{y}$ with the corresponding errors $\varepsilon_{\mathbf{x}}$ and $\varepsilon_{\mathbf{y}}$, i.e. $\|\mathbf{x} - \underline{\mathbf{x}}\|_\nu \leq \varepsilon_{\mathbf{x}}$ and $\|\mathbf{y} - \underline{\mathbf{y}}\|_\nu \leq \varepsilon_{\mathbf{y}}$. Let us describe the common operations

Op.	Approximation	Bounded Error
$\mathbf{x} + \mathbf{y}$	$\underline{\mathbf{x} + \mathbf{y}} = \underline{\mathbf{x}} + \underline{\mathbf{y}}$	$\varepsilon_{\mathbf{x}+\mathbf{y}} = \varepsilon_{\mathbf{x}} + \varepsilon_{\mathbf{y}}$
$\mathbf{x} * \mathbf{y}$	$\underline{\mathbf{x} * \mathbf{y}} = \underline{\mathbf{x}} * \underline{\mathbf{y}}$	$\varepsilon_{\mathbf{x}*\mathbf{y}} = \|\underline{\mathbf{x}}\|_\nu \varepsilon_{\mathbf{y}} + \|\underline{\mathbf{y}}\|_\nu \varepsilon_{\mathbf{x}} + \varepsilon_{\mathbf{x}} \varepsilon_{\mathbf{y}}$
$\mathbf{x}^{-1}$	$\underline{\mathbf{x}^{-1}} = \mathbf{a} \in \ell^1_\nu$ s.t. $\|\underline{\mathbf{x}} * \mathbf{a} - \mathbf{1}\|_\nu + \|\mathbf{a}\|_\nu \varepsilon_{\mathbf{x}} < 1$	$\varepsilon_{\mathbf{x}^{-1}} = \|\mathbf{a}\|_\nu \dfrac{\|\underline{\mathbf{x}} * \mathbf{a} - \mathbf{1}\|_\nu + \|\mathbf{a}\|_\nu \varepsilon_{\mathbf{x}}}{1 - \|\underline{\mathbf{x}} * \mathbf{a} - \mathbf{1}\|_\nu - \|\mathbf{a}\|_\nu \varepsilon_{\mathbf{x}}}$

Let $\bar{\mathbf{v}} \in \ell^1_\nu$ finite (i.e. $\underline{\bar{\mathbf{v}}} = \bar{\mathbf{v}},\ \varepsilon_{\bar{\mathbf{v}}} = 0$). Let $\mathbf{v} \in \mathcal{B}_\nu(\bar{\mathbf{v}}, r)$, we can see $\mathbf{v}$ as $\underline{\mathbf{v}} = \bar{\mathbf{v}}$ and $\varepsilon_{\mathbf{v}} = r$.

Let f be an entire function, $f(x) = \sum_{k=0}^{+\infty} a_k x^k$.

Approximation: $$\underline{f(\bar{\mathbf{v}})} = \sum_{k=0}^{K-1} a_k \bar{\mathbf{v}}^{*k}$$

Error bound: $$\varepsilon_{f(\bar{\mathbf{v}})} = \frac{\|\bar{\mathbf{v}}\|_\nu^K}{K!} \sup_{\mathbf{z}\in[\mathbf{0},\bar{\mathbf{v}}]} \|f^{(K)}(\mathbf{z})\|_\nu$$

Local bound: $$\|f(\mathbf{v})\|_\nu \leq \|\underline{f(\bar{\mathbf{v}})}\|_\nu + \varepsilon_{f(\bar{\mathbf{v}})} + |f'|(\|\bar{\mathbf{v}}\|_\nu + r)r$$

With such tools, we can manage any product and division of any power series or polynomials!

NB: $|g|(x) = \sum_{k=0}^{+\infty} |b_k| x^k$ where $g(x) = \sum_{k=0}^{+\infty} b_k x^k$

$\gamma(x)$	$\dfrac{1}{1+x^9}$	$1+\exp(9(x-1))$
$\underline{\gamma(\bar{\mathbf{v}})}$	$\underline{(\mathbf{1}+\bar{\mathbf{v}}^{*9})^{-1}} := \mathbf{a}$	$\mathbf{1}+\sum_{k=0}^{K-1}\dfrac{9^k}{k!}(\bar{\mathbf{v}}-\mathbf{1})^{*k}$
$\varepsilon_{\gamma(\bar{\mathbf{v}})}$	$\Vert\mathbf{a}\Vert_\nu \dfrac{\Vert\mathbf{a}*(\mathbf{1}+\bar{\mathbf{v}}^{*9})-\mathbf{1}\Vert_\nu}{1-\Vert\mathbf{a}*(\mathbf{1}+\bar{\mathbf{v}}^{*9})-\mathbf{1}\Vert_\nu}$	$\dfrac{9^K\Vert\bar{\mathbf{v}}-\mathbf{1}\Vert_\nu^K}{K!}\exp(9\Vert\bar{\mathbf{v}}-\mathbf{1}\Vert_\nu)$

And the local bounds:

$$\Vert(\mathbf{1}+\mathbf{v}^{*9})^{-1}\Vert_\nu \leq \Vert\mathbf{a}\Vert_\nu + \Vert\mathbf{a}\Vert_\nu \frac{\Vert\mathbf{a}*(\mathbf{1}+\bar{\mathbf{v}}^{*9})-\mathbf{1}\Vert_\nu + \Vert\mathbf{a}\Vert_\nu r}{1-\Vert\mathbf{a}*(\mathbf{1}+\bar{\mathbf{v}}^{*9})-\mathbf{1}\Vert_\nu - \Vert\mathbf{a}\Vert_\nu r}$$

$$\Vert\mathbf{1}+\exp(9(\mathbf{v}-\mathbf{1}))\Vert_\nu \leq \Vert\underline{\gamma(\bar{\mathbf{v}})}\Vert_\nu + \varepsilon_{\gamma(\bar{\mathbf{v}})} + 9\exp(9(\Vert\bar{\mathbf{v}}-\mathbf{1}\Vert_\nu + r))r$$

We have to express all the bounds with just what the computer can know.

$$F(\overline{\mathbf{U}}) = \begin{pmatrix} \Delta(\gamma(\bar{\mathbf{v}}) * \bar{\mathbf{u}}) + \sigma\bar{\mathbf{u}} * (\mathbf{1} - \bar{\mathbf{u}}) \\ \\ d\Delta\bar{\mathbf{v}} + \bar{\mathbf{u}} - \bar{\mathbf{v}} \end{pmatrix},$$

$$Y = \underbrace{\left\|A\underline{F(\overline{\mathbf{U}})}\right\|_\nu}_{\text{finite part}} + \overbrace{(\left\|A^{11}\Delta\right\|_\nu + \left\|A^{21}\Delta\right\|_\nu)\,||\bar{\mathbf{u}}||_\nu \quad \times \quad \underbrace{\varepsilon_{\gamma(\bar{\mathbf{v}})}}_{\text{error on } \gamma}}^{\text{outcome of the operation on the rests}} .$$

For more details look at [BP23].

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4. Are (7a-b), (8) satisfied? Conclude.

Theorem (Validation of Figure 2)

*Let $\sigma = 0.053$, $d = 1$, $l = 3\pi$ and $\gamma(x) = \frac{1}{1+x^9}$. Let $(\bar{u}, \bar{v})$ the functions described in **Figure 2**. There exists a smooth steady states (u, v) of the 'K-S equation' (1), such that* $\sup_{[0,l]} |u - \bar{u}| + \sup_{[0,l]} |v - \bar{v}| \leq 2.5199 \times 10^{-8}$.

Let $N = 100$, $\nu = 1.0001$ and $r^* = 1 \times 10^{-6}$. With the toolbox and some calculations (made by hand and by the computer with MATLAB and `intlab`). We have $Y = 2.4052 \times 10^{-8}$, $Z_1 = 3.1193 \times 10^{-2}$ and $Z_2 = 3.6099 \times 10^{4}$. They satisfy the hypothesis of the 'N-K Theorem'. We have the existence and uniqueness of (u, v) with $r = 2.5199 \times 10^{-8}$.

Theorem (Validation of Figure 3)

Let $\sigma = 0.6$, $d = 1$, $l = 4\pi$ *and* $\gamma(x) = \dfrac{1}{1+\exp(9(x-1))}$. *Let* $(\bar{u}, \bar{v})$ *the functions described in* ***Figure 3***. *There exists a smooth steady states* (u, v) *of* (1),
such that $\sup_{[0,l]} |u - \bar{u}| + \sup_{[0,l]} |v - \bar{v}| \leq 1.6956 \times 10^{-12}$.

This result corroborates with [WX21]. It affirms the existence of theoretical solution of their numerical solution.

Let $N = 100$, $\nu = 1.0001$ and $r^* = 1 \times 10^{-6}$. With the toolbox and some calculations (made by hand and by the computer with MATLAB and `intlab`). We have $Y = 1.5327 \times 10^{-12}$, $Z_1 = 2.4338 \times 10^{-2}$ and $Z_2 = 6.4843 \times 10^{2}$. They satisfy the hypothesis of the 'N-K Theorem'. We have the existence and uniqueness of (u, v) with $r = 1.6956 \times 10^{-12}$.

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Conclusion

- ⋆ The computer assisted proof method is consistent and efficient. We have theorems of existence of solutions to the stationary problem (2). And a (very) close approximation of solution.

- ⋆ We can systematise the process of obtaining a solution. see [BP23]

- ⋆ We have developed (and are developing) a technique, a toolbox, to manage non-polynomial terms.

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- ⋆ Gain speed in all calculations. Develop the code, to improve performance and enable increasingly complex operations.
- ⋆ All this is being worked on with Olivier Hénot and Maxime Breden.

Thanks for your attention!

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