Parabolic models for chemotaxis on weighted networks

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Overview

- A mathematical model for chemotaxis: the Keller-Segel system
- Chemotaxis on networks and the role of transmission conditions
- The heat equation and the heat kernel on weighted networks
- Global existence of a solution for the Keller-Segel system on networks
- Conclusions and perspectives

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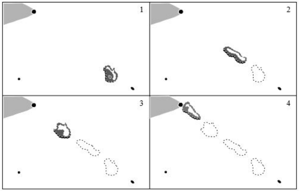
The Chemotaxis model

One of the most important self-organization process is the **Chemotaxis** ($\tau\alpha\xi\iota\varsigma$=arrangement, disposition).

In a collective motion of a population of micro-organisms (a single-cell or a multicellular organism), a single cell which reaches a place where it can consume food or reproduce emits a chemo-attractant signal which attracts the rest of the population walk.



(a)

biased random walk of a cell

The Keller-Segel system in the Euclidean space

There are several models for chemotaxis. Choosing a macroscopic description of the population, considering uniquely the cell density $u \geq 0$ and the chemical concentration $c \geq 0$ and assuming that

- cells move randomly and are attracted by the chemical signal;
- the chemical is produced by the cells themselves;
- the population is conserved

a corresponding mathematical model is given by the density and concentration balance equations [Keller-Segel, 1970]

$$u_t = \Delta u - \nabla \cdot (u \nabla c)$$

$$\varepsilon c_t = \Delta c + u - \alpha\, c$$

ε, α non negative coefficients(if $\varepsilon > 0$ parabolic-parabolic system; if $\varepsilon = 0$ elliptic-parabolic system) plus initial/boundary condition

There is a huge quantity of literature on the mathematical analysis of the Keller-Segel system (for review papers, see [*Horstmann 2003*], [*Hillen-Painter 2009*]).
Nevertheless, several challenging issues are still open. Depending on the space dimension, on $\varepsilon \geq 0$ and on the initial mass $\int u_0(x)dx$ different phenomena can occur . Roughly speaking :

- dim 1: Solutions are global and bounded
- dim 2: Threshold phenomenon for a critical value $\overline{M}$ of the initial mass: global existence for $\int u_0(x)dx < \overline{M}$, possible blow-up for $\int u_0(x)dx \geq \overline{M}$.
- dim 3: local existence and possible blowup in finite time for any initial mass

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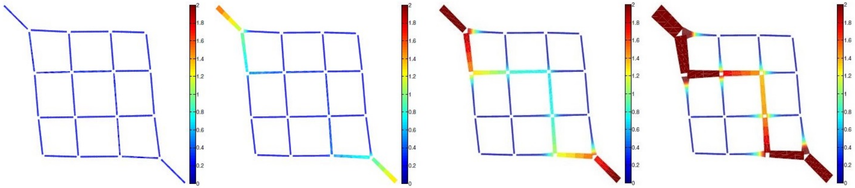
In [Borsche, Göttlich, Klar, Schillen 2014], the authors consider a parabolic model for chemotaxis on network to simulate the behaviour of the Physarum polycephalum (a hyperbolic model is studied in [Guarguaglini-Natalini 2015])

- A Keller-Segel system is introduced on each arc with some transition conditions at the vertices;
- The Keller-Segel system is discretized and numerical experiments show that it is able to capture the behavior of the Physarium



(a) Time = 0 (b) Time = 1 (c) Time = 5 (d) Time = 10

Our aim is to study the well-posedness of the continuous Keller-Segel system on the network.

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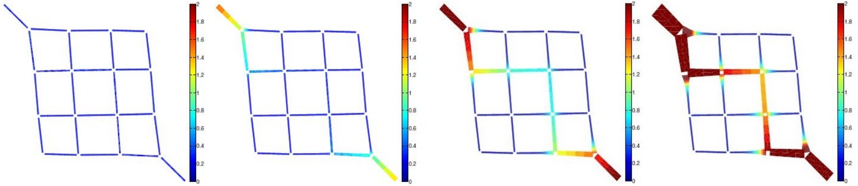
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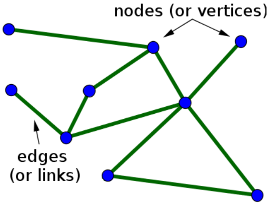
The network

- $V := \{v_1, \dots, v_n\}$ the finite set of vertices in $\mathbb{R}^N$
- $E := \{e_1, \dots, e_m\}$ the finite set of edges (curves in $\mathbb{R}^N$) whose endpoints are vertices
- $\Gamma := (V, E)$ the finite connected network
- each edges is parametrized by two homeomorphisms $\Pi_j^{\pm} : [0, 1] \mapsto \mathbb{R}$ which give rise to two oriented arcs $e_j^{\pm}$
- to each edge $e_j \in E$ is associated a positive weight $\kappa(e_j) > 0$ (the network is not homogeneous)
- $E(v_i) := \{j \ : \ e_j$ is incident to $v_i \in V\}$



Integral and derivatives on Γ

- A function $u : \Gamma \to \mathbb{R}$ is a collection of m functions $(u_j)_{j=1}^m$ defined on the arcs, i.e. $u_j := u_{|_{\bar{e}_j}}$
- The derivative $u_j'(x)$ is always intended with respect to the parametrization, i.e. $(u \circ \Pi_j^{\pm})'(t)$ for $x = \Pi_j^{\pm}(t) \in e_j$
- At the vertices we defined the *exterior normal derivative*

$$\frac{\partial u_j}{\partial n}(I(a_j)) = -\lim_{h \to 0^+} \frac{(u \circ \Pi_j^{\pm})(h) - (u \circ \Pi_j^{\pm})(0)}{h}$$

$$\frac{\partial u_j}{\partial n}(T(a_j)) = \lim_{h \to 0^-} \frac{(u \circ \Pi_j^{\pm})(1 + h) - (u \circ \Pi_j^{\pm})(1)}{h}$$

  with $I(a_j)$ and $T(a_j)$ the initial and terminal endpoint of a_j resp.
- Also the integrals are computed in the parameters, i.e.

$$\int_\Gamma u(x)\, dx = \sum_{j=1}^m \kappa(e_j) \int_0^1 (u \circ \Pi_j^{\pm})(t)\, dt$$

The Keller-Segel system on the network Γ

The Keller-Segel system

$$\partial_t u = \nabla \cdot (\nabla u - u \nabla c)$$
$$\varepsilon\, \partial_t c = \Delta c + u - \alpha\, c$$

translates into m systems (one for each edge e_j)

$$\partial_t u_j = \partial_{xx} u_j - \partial_x (u_j\, \partial_x c_j) \qquad \text{on } e_j \times (0, \infty)\,,\ j = 1, \dots, m,$$
$$\varepsilon\, \partial_t c_j = \partial_{xx} c_j + u_j - \alpha\, c_j \qquad \text{on } e_j \times (0, \infty)\,,\ j = 1, \dots, m,$$

What about the conditions at the vertices?

Boundary and transmission conditions

- In the (boundary vertices) $\partial\Gamma := \{v_{i_1}, \ldots, v_{i_k}\} \subset V$, $0 \leq i_k \leq n$, i.e. vertices with a single incident arc, we assume that the fluid just flows in or out. Hence on $\partial\Gamma$ we consider Neumann conditions

$$\frac{\partial u_j}{\partial n}(t, v_i) = \frac{\partial c_j}{\partial n}(t, v_i) = 0\,, \qquad v_i \in \partial\Gamma$$

- The remaining vertices are the transition vertices $V_T := V \setminus \partial\Gamma$ At the transition vertices we assume continuity of the solutions

$$u_j(t, v_i) = u_k(t, v_i), \qquad c_j(t, v_i) = c_k(t, v_i), \quad j, k \in E(v_i),$$

and the Kirchhoff conditions

$$\sum_{j \in E(v_i)} \kappa(e_j) \frac{\partial u_j}{\partial n}(t, v_i) = \sum_{j \in E(v_i)} \kappa(e_j) \frac{\partial c_j}{\partial n}(t, v_i) = 0.$$

Remark

- Continuity of the solutions and the Kirchhoff conditions are the simplest conditions for the validity of the **Maximum Principle** for linear differential operator on networks.
- The transition conditions for u, c implies the conservation of the total flux at the vertices. Indeed by the continuity of u at vertices and the Kirchhoff conditions for u and c, we have

$$\sum_{j \in E(v_i)} \kappa(e_j) \left[\frac{\partial u_j}{\partial n} - u_j \frac{\partial c_j}{\partial n} \right] (t, v_i) = 0 \,, \qquad t > 0, \; i = 1, \ldots, n \,.$$

- The transition conditions guarantee the conservation of the initial mass, i.e.

$$\int_\Gamma u(t,y)\, dy = \int_\Gamma u^0(y)\, dy \quad \forall t > 0$$

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Summarizing we consider the Keller-Segel system

$$\partial_t u_j = \partial_{yy} u_j - \partial_y (u_j \, \partial_y c_j) \qquad j = 1, \dots, m,$$

$$\varepsilon \, \partial_t c_j = \partial_{yy} c_j + u_j - \alpha \, c_j \qquad j = 1, \dots, m,$$

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Our aim is to show the well-posedness of the previous problem. Since the problem on each arc is 1-dimensional we expect to get global, bounded solutions.

In $\mathbb{R}$ this result was proved in [Hillen-Potapov, 2004] by means of:

- Decay estimates in time for the heat kernel in $\mathbb{R}$
- Duhamel formula for the solution of the Keller-Segel system
- Careful application of interpolation inequalities in Sobolev space

The Heat equation

$$\begin{cases} \partial_t u_j = \partial_{xx} u_j & \text{on } (0,\infty) \times e_j\,,\ j = 1,\dots,m \\ u_j(0,x) = f_j(x) & \text{on } e_j\,,\ j = 1,\dots,m \\ u_j(t,v_i) = u_k(t,v_i) & \text{if } j,k \in E(v_i),\ v_i \in V \\ \sum_{j \in E(v_i)} \kappa(e_j) \frac{\partial u_j}{\partial n}(t,v_i) = 0\,, & v_i \in V \end{cases}$$

(for simplicity assume that Γ has no boundary points).

The existence of a solution to the heat equation has been obtained in

- Variational methods [Lumer 1980, Nicaise 1987];
- Heat kernel [Roth, 1984];
- Probabilistic methods [Freidlin-Wentzell, 1993];
- Abstract semigroup approach [Mugnolo, 2007].

All these approaches are equivalent, but the explicit formula for the Heat kernel in Roth is fundamental to obtain decay estimates

The heat kernel formula

Paths and distance on networks

- $C_k(x,y) := \{C = (e_{j_1}, \ldots, e_{j_k}) \ : \ x \in e_{j_1} \text{ and } y \in e_{j_k}\}$, $k = 2, 3, \ldots$, denotes the set of paths of length k such that x belongs to the first arc and y to the last one
- A geodesic path joining x to y on Γ is any path of minimum length in $\cup_{k \geq 2} C_k(x,y)$.
- $\mathcal{L}(x,y) \in \mathbb{N}$ denotes the number of arcs of a geodesic path joining x to y
- The distance $d_C(x,y)$ between x and y along the path $C = (e_{j_1}, \ldots, e_{j_k})$ is given by
  - (i) $d_C(x,y) = |(\Pi_j^{\pm})^{-1}(x) - (\Pi_j^{\pm})^{-1}(y)|$ if $x, y \in \overline{e}_j$;
  - (ii) $d_C(x,y) = d_C(x, T(e_{j_1})) + d_C(y, I(e_{j_k})) + |C| - 2$
- $\varepsilon(C)$ represents the total weight of a path $C \in C_k$

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The Heat kernel

For $t > 0$, $x \in e_i$, $y \in e_j$, define

$$H(t,x,y) = \delta_{i,j}\,\kappa^{-1}(e_i)\,G(t,d_C(x,y)) + L(t,x,y)$$

where

- $\delta_{i,j}$: the usual Kronecker's delta function
- $G(t,z) = \frac{1}{\sqrt{4\pi\,t}} e^{-\frac{z^2}{4t}}$
- $L(t,x,y) = \sum_{k \geq \mathcal{L}(x,y)} \sum_{C \in C_k(x,y)} \kappa^{-1}(e_i)\,\varepsilon(C)\,G(t,d_C(x,y))$

The first term G is simply the restriction of the fundamental solution of the heat equation on each edge of the network.
The second term L takes into account the instantaneous propagation of the heat along all the possible infinite many paths joining x to y on the network (in a path, a same arc can be passed through several times).

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Theorem (Roth)

Let H be the heat kernel on the network Γ. Then

1. *H is continuous on $(0, \infty) \times \Gamma \times \Gamma$;*
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Corollary

For all $f \in C^0(\Gamma)$, *the function*

$$P_t f(y) = (H(t) * f)(y) := \int_\Gamma H(t,x,y) f(x) dx, \qquad (t,y) \in (0,\infty) \times \Gamma$$

with $P_0 f = f$ *is the unique continuous solution of the Cauchy problem*

$$\begin{cases} \partial_t u_j = \partial_{xx} u_j & \text{on } (0,\infty) \times e_j\,,\ j = 1,\dots,m \\ u_j(0,x) = f_j(x) & \text{on } e_j\,,\ j = 1,\dots,m \\ u_j(t,v_i) = u_k(t,v_i) & \text{if } j,k \in E(v_i),\ v_i \in V \\ \sum_{j \in E(v_i)} \kappa(e_j) \frac{\partial u_j}{\partial n}(t,v_i) = 0\,, & v_i \in V \end{cases}$$

The specific form of the transition conditions at the vertices

$$u_j(t, v_i) = u_k(t, v_i) \qquad j, k \in E(v_i),\ i = 1, \ldots, n,\ t > 0$$

$$\sum_{j \in E(v_i)} \kappa(e_j) \frac{\partial u_j}{\partial n}(t, v_i) = 0 \qquad i = 1, \ldots, n,\ t > 0$$

allows to write the solution of the heat equation in the integral form

$$P_t f(y) = (H(t) * f)(y) := \int_\Gamma H(t, x, y) f(x) dx, \qquad (t, y) \in (0, \infty) \times \Gamma$$

since in the integration by parts on the arcs the boundary terms cancels with the conditions at the vertices.

Proposition (Optimal decay estimates)

Let H be the heat kernel on Γ. Then,

$$\int_\Gamma H(t,x,y)dy = 1\,, \qquad \forall\,(t,x) \in \Gamma \times (0,\infty)\,,$$

and there exist constants $C_i > 0$, $i = 1,\dots,4$, such that for all $t > 0$ it holds

$$\sup_{x\in\Gamma} \|H(t,x,\cdot)\|_{L^1(\Gamma)} \le C_1\,,$$

$$\|H(t)\|_{L^\infty(\Gamma\times\Gamma)} \le C_2(1 + t^{-1/2})\,,$$

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(by simmetry the above properties holds changing x with y).

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Integral solutions of Keller-Segel system

By Duhamel formula, we consider solutions of the Keller-Segel system in integral form

$$u(t,y) = P_t u^0(y) - \int_0^t P_{(t-s)}[\partial_x(u(s)\partial_x c(s))](y)ds$$

$$c(t,y) = e^{-(\alpha/\varepsilon)t} P_{(t/\varepsilon)} c^0(y) + \frac{1}{\varepsilon}\int_0^t e^{-(\alpha/\varepsilon)(t-s)} P_{((t-s)/\varepsilon)}\left[u(s)\right](y)ds$$

where P_t is the semigroup generated by the heat equation on Γ, i.e. for an integrable function f

$$P_t f(y) = (H(t) * f)(y) := \int_\Gamma H(t,x,y) f(x) dx, \qquad (t,y) \in (0,\infty) \times \Gamma$$

From now on we will refer to the previous formulas as the integral solutions of the Keller-Segel system.

The parabolic-parabolic Keller-Segel system ($\varepsilon > 0$)

Theorem (Local existence)

Assume $u^0 \in L^\infty(\Gamma)$, $c^0 \in W^{1,\infty}(\Gamma)$. Then, there exist $T = T(\|u^0\|_{L^\infty(\Gamma)}, \|\partial_x c^0\|_{L^\infty(\Gamma)}, \varepsilon) > 0$ and a unique integral solution (u, c) of the Keller-Segel system with

$$u \in L^\infty((0,T); C^0(\Gamma)), \quad c \in L^\infty(0,T; W^{1,\infty}(\Gamma)),$$

satisfying the transmission conditions and the mass conservation.

The proof is based on a fixed point argument and makes use in a crucial way of the decay estimates on the heat kernel

Since the time T depends only on the initial data, by means of a continuation method we can prove that

Theorem (Global existence and positivity)

Assume $u^0 \in L^\infty(\Gamma)$, $c^0 \in W^{1,\infty}(\Gamma)$. Then for all $T > 0$ there exists a solution (u, c) of the Keller-Segel system on the time interval $[0, T]$. Moreover, if the initial data u^0 and c^0 are nonnegative, the solution (u, c) is nonnegative.

In conclusion, the main points of our approach to well-posedness of Keller-Segel system are

- Heat kernel and integral formula for the heat equation on networks
- Optimal decay estimates for the heat kernel
- Duhamel formula for the inhomogeneous heat equation on networks

In all the previous points the transmission conditions at the vertices plays a crucial role.

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Conclusions

- Existence and uniqueness of the solution to the parabolic-parabolic Keller-Segel system in $[0, T]$ for any time $T > 0$, but it is not excluded blow-up for $T \to +\infty$.
- Existence and uniqueness of the solution to the elliptic-parabolic Keller-Segel system in $[0, \infty)$

Perspectives

- Asymptotic behavior of the solution for $T \to \infty$ (existence of an asymptotic profile has been observed numerically in [Hillen-Potakov, 2004])
- Convergence of the numerical scheme developed in [Borsche, Göttlich, Klar, Schillen 2014] (slightly different transmission conditions)
- Behavior of the solutions with respect to the structural elements of the network
- Optimal decay estimates of the Heat kernel for other problems of parabolic nature on networks.

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