Enhancement of biological reaction by chemotaxis

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Broadcast spawning for aquatic animals

- Broadcast spawning is a fertilization strategy used by sea urchins, corals, etc.

  1. Males and females release sperm and egg gametes into the surrounding flow.
  2. The gametes are buoyant and rise to the surface of the ocean.
  3. The fertilized gametes form larvae, which go down to the bottom of the ocean to start a new colony.

- The gametes might be initially far apart from each other, but the fertilization rate for corals are often as high as 90%.

- What causes this high fertilization rate?

Possible explanations

- The effective diffusion caused by turbulent flow might help. But it also dilutes the gametes, and numerical simulation based on this predict fertilization rates of less than 1%.
- Crimaldi et al. ('06) showed that vortex stirring can generally enhance the reaction rate.
- Chemotaxis may play a role in coral fertilization too, since eggs release a chemical that attracts sperm.
- The following one-density simplified model is proposed by Kiselev and Ryzhik ('12),

$$\rho_t = \Delta\rho + \nabla \cdot (\rho\nabla(\mathcal{N} * \rho)) - \epsilon\rho^2,$$

and they showed that chemotaxis indeed enhances reaction rate.

A chemotaxis model with two densities

- Below is a minimal model to describe the reaction between the sperm density ρ_1 and egg density ρ_2 in $\mathbb{R}^2$:

$$\begin{cases} \partial_t \rho_1 = \Delta \rho_1 + \nabla \cdot (\rho_1 \nabla (\mathcal{N} * \rho_2)) - \epsilon \rho_1 \rho_2 \\ \partial_t \rho_2 = -\epsilon \rho_1 \rho_2, \end{cases}$$

where $\mathcal{N} = \frac{1}{2\pi} \ln |x|$ is the Newtonian potential in $\mathbb{R}^2$.

- The difference to Keller-Segel equation: Here ρ_1 is attracted by the chemical released by ρ_2, rather than by itself.

- It is somewhat similar to the systems studied by Othmer-Stevens ('97), Corrias-Perthame-Zaag('04):

$$\begin{cases} \partial_t n = \Delta n - \nabla \cdot (n \chi(c) \nabla c) \\ \partial_t c = -nc, \end{cases}$$

- Global existence for our system almost comes for free. But does the chemotaxis term indeed enhance reaction between ρ_1 and ρ_2?

- Assume that $\|\rho_{02}\|_1 = \gamma$, $\|\rho_{02}\|_\infty \sim \gamma$, and ρ_{02} is initially supported in the unit ball $B(0,1)$.
- Assume that $\|\rho_{01}\|_1 = M$, where $M \gg \gamma \gg 1$. Suppose initially ρ_{01} and ρ_{02} are separated by distance $L \gg 1$.
- For the reaction rate ϵ, assume $\epsilon \ll 1$.

Chemotaxis v.s. pure diffusion: Heuristics

- Let τ denote the "half time" of ρ_2, i.e. τ is the time it takes so that the L^1 norm of ρ_2 drop by a half. (i.e. a half of the eggs become fertilized)

- With chemotaxis, note that the drift velocity term at x is given by $\nabla(\mathcal{N} * \rho_2)(x)$, which is of order $\gamma/|x|$ before the half-time is reached.

$$\nabla(\mathcal{N} * \rho_2) \geq \gamma/L$$

mass γ
$\gamma \gg 1$

ρ_2 ρ_1

$L \gg 1$
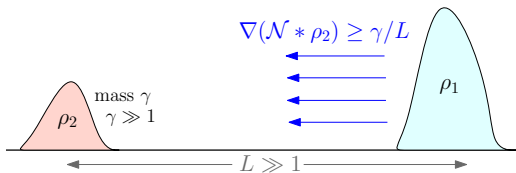
- As a result, within time $L/(\gamma/L) = L^2/\gamma$, a significant portion of ρ_1 will be bring into the unit ball, and the reaction will be quick since we assume $M\epsilon \gg 1$.

- It suggest that with chemotaxis term, $\tau \lesssim \dfrac{L^2}{\gamma}$.

Comparing the formal estimate $\tau \lesssim \frac{L^2}{\gamma}$ (chemotaxis case) with $\tau \geq \frac{L^2}{4\ln(M\epsilon)}$ (pure diffusion case), we expect that the chemotaxis term would enhance reaction for $1 \ll M\epsilon \ll e^\gamma$.

We are able to prove a slightly weaker result:

Theorem

Given that $M\epsilon \gg \gamma$, if ρ_{01}, ρ_{02} are both radially symmetric, with $\|\rho_{01}\|_1 = M$, ρ_{01} initially concentrated around distance L from 0, and $\rho_2 = \gamma\chi_{B(0,1)}$. Then the half time τ for the chemotaxis system satisfies

$$\tau \lesssim \log\gamma + \frac{L^2}{\gamma}.$$

Mass comparison

- Assume for contradiction that $\tau \gg \log \gamma + L^2/\gamma$.
- We want to show by this time, a significant portion of ρ_1 has moved into a ball smaller than B_1, thus eating a large part of ρ_2 and causing a contradiction.
- Idea: For all $t \leq \tau$, $\rho_2(\cdot, t)$ is always "more attracting" than the following function g:(i.e. $|\partial_r(\mathcal{N} * \rho_2(\cdot, t))| \geq |\partial_r(\mathcal{N} * g)|$)

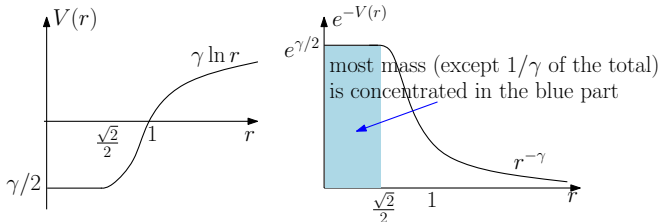$$g = \gamma 1_{B_1 \setminus B_{\sqrt{2}/2}}.$$

- Thus by fixing $\rho_2 = g$ (and ignore the reaction term for ρ_1), if we can show that most mass of ρ_1 move into the ball by time $\log \gamma + L^2/\gamma$, for the real system this must be true as well!

A detour to Fokker-Planck equation

- For $g = \gamma 1_{B_1 \setminus B_{\sqrt{2}/2}}$, consider the Fokker-Planck equation with potential $V(x) := \mathcal{N} * g$:
$$\rho_t = \Delta \rho + \nabla \cdot (\rho \nabla V).$$

- It is well known that Ce^{-V} is the unique stationary solution to this equation.

- For this stationary solution Ce^{-V}, it is easy to check that most of its mass is in $B_{\sqrt{2}/2}$.

- Question: Does every solution converge to Ce^{-V} as $t \to \infty$? If so, at what rate?

Previous results on convergence rate of Fokker-Planck eq

- For convex V, there are many results regarding the convergence rate:

  - If $D^2 V \geq \lambda \, Id$ (with $\lambda > 0$), then ρ converges to Ce^{-V} in $L^2(e^V)$ exponentially fast. (Bakry-Emery '85)

  - Also, in this case contraction results in 2-Wasserstein distance hold between any two solutions, and in particular $W_2(\rho, Ce^{-V}) \lesssim e^{-\lambda t}$. (Carrillo-McCann-Villani '03)

  - For $V = |x|^{\alpha}$ with $1 \leq \alpha < 2$ (where V is convex but not uniformly convex), solution also converges with exponential rate. (Arnold-Markowich-Toscani-Unterreiter '04)

- Bad news: our V is not convex!
  (V is convex for $r < 1$, but
  $V = \gamma \ln r$ for $r > 1$).
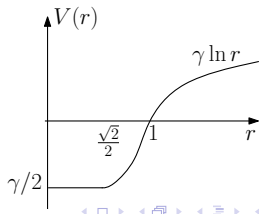
L^2 estimates on Fokker-Planck equation

- WLOG assume $\int \rho = \int e^{-V} = 1$, and let $f = \rho e^V$. Consider

$$F(t) := \int (\rho - e^{-V})^2 e^V dx = \int (f-1)^2 e^{-V} dx.$$

- One can check that F is non-increasing in time, since

$$F'(t) = -\int |\nabla f|^2 e^{-V} dx \leq 0.$$

- For $D^2 V \geq \lambda Id$ $(\lambda > 0)$, logarithmic Sobolev inequality gives $\int |\nabla f|^2 e^{-V} dx \geq \lambda \int (f-1)^2 e^{-V} dx$, implying $F'(t) \leq -\lambda F$.

- For $e^{-V} = \frac{1}{Z}(1 + |x|^2)^{-\gamma/2}$, Bobkov-Ledoux ('09) has the following weighted Poincaré's inequality:

$$\int (f-1)^2 e^{-V} dx \lesssim \frac{1}{\gamma} \int |\nabla f|^2 (1 + |x|^2) e^{-V} dx$$

A new weighted Poincaré's inequality

- This weighted Poincaré's inequality is sharp, but it would not give us the optimal decay rate for $F(t)$.
- We thus take advantage of the fact that V is flat in $B_{\sqrt{2}/2}$, and derive another sharp weighted Poincaré's inequality as follows:

$$\int (f-1)^2 e^{-V} dx \lesssim \int_{B_1} |\nabla f|^2 e^{-V} dx + \frac{1}{\gamma^2} \int_{B_1^c} |\nabla f|^2 |x|^2 e^{-V} dx$$

- This eventually gives us an optimal decay estimate for $F(t)$:

$$F'(t) \lesssim -\min\left\{F(t), \gamma^{\frac{2(\gamma-2)}{\gamma-4}} \|f\|_{L^\infty}^{-\frac{8}{\gamma-4}} F(t)^{\frac{\gamma}{\gamma-4}}\right\}.$$

- To go from L^2 to L^1, we then use a duality argument to obtain a decay estimate for $\|\rho(\cdot, t) - e^{-V}\|_{L^1}$, which says the L^1 difference must be small by time $\log \gamma + \frac{L}{\gamma^2}$.

Problem with non-radial initial data

- If $\rho_1(\cdot, 0)$ and $\rho_2(\cdot, 0)$ are nonradial, chemotaxis may actually slow down reaction rate!

- Consider the following example in 1D (with 1D Newtonian potential $|x|$), where $\gamma \gg 1$:
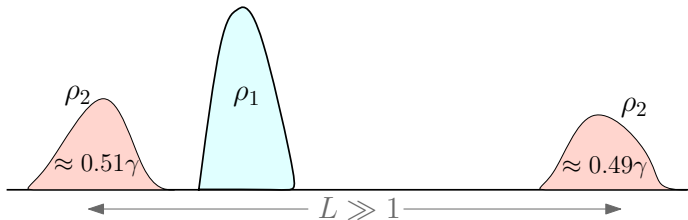
- One can extend this example to 2D by extending the initial data on y axis (and truncate it for y sufficiently large).

Thank you for your attention!