Gradient Ascent in Chemotaxis

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1. Introduction to Chemotaxis

Chemotaxis is a phenomenon in nature in which single-celled and multi-celled organisms base their movements according to a chemical concentration gradient that is either toward or away from the chemical stimulus. Chemotaxis is considered to be one of the most researched areas in the study of cell migration. The specific Chemotaxis model we are looking at deals with the movement of an $n \epsilon \mathbb{N}$ amount of organisms towards a material or source of food due to a chemical stimulus. The model for this problem is described by the density of the material and the position of the organisms. We will denote the density of the material by a function c(x, y, t) and the position of the organisms by a vector $X_k(t)$, with t representing time. Our model is the following:

$$\begin{cases} \dfrac{\partial c}{\partial t} = \delta \Delta c - r(c) \displaystyle\sum_{k=1}^{n} f(X_k(t)), & \delta, r(c) \epsilon \mathbb{R} \\ \dot{X}(t) = \rho \nabla c\big(X_k(t)\big) + N_t, & \rho \epsilon \mathbb{R} \end{cases}$$

where δ is the diffusion coefficient, r(c) is the rate at which the organisms consume the material, ρ is the velocity at which the organisms move, f is a function that describes how the organisms consume the material, and where N_t is a noise term, which we constructed out of a random number generator. The first equation presented above describes the change in the density of the material which depends on the rate at which the material diffuses, represented δ, and the manner the in which the organisms consume the material. The second equation describes the movement of the organisms towards the material or chemical stimulus with N_t describing the tumbling of the organisms as they approach the chemical stimulus.

The problem we are dealing with in our Chemotaxis model is seeking the gradient ascent for the model, which is the direction in which $\dot{X}(t)$ increases most rapidly over time. Geometrically, the gradient ascent is the steepest uphill direction of our model and it can be interpreted as the direction or path in which the organisms reach the chemical stimulus the fastest. We will be looking for the gradient ascent in two cases. The first case will consider the model without the noise term, N_t, and the second case will look at the change that occurs in the gradient ascent when the noise term is included. For both cases, we solved the model by applying taylor expansions.

2. Chemotaxis (with diffusion)

When implementing the model for the first case, we end up with the results displayed in the following figures

Figure A1

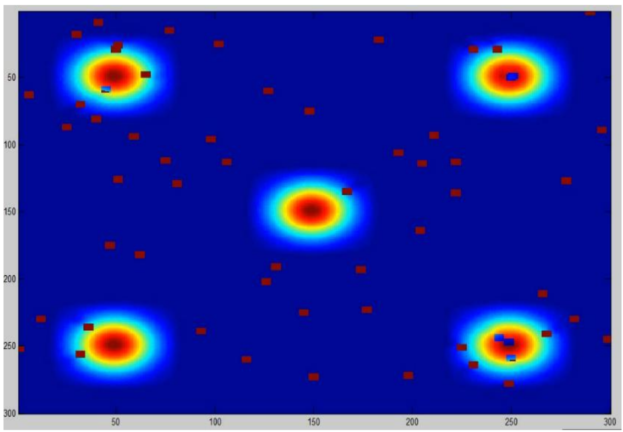


Figure A2

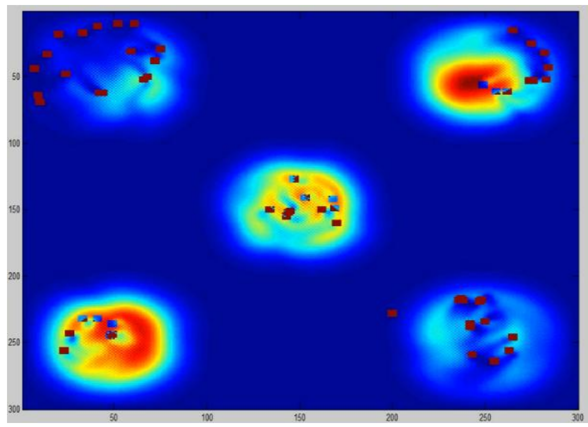


Figure A3

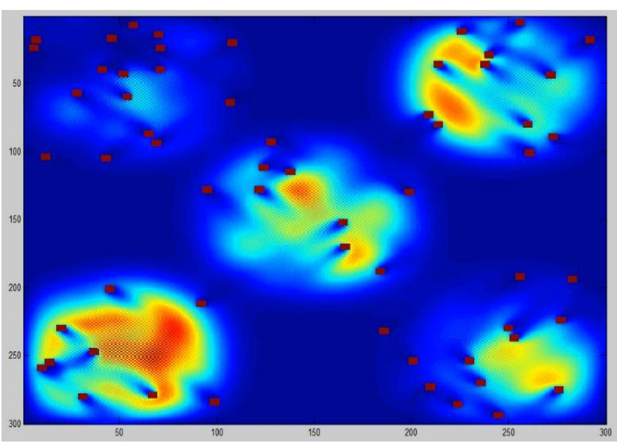
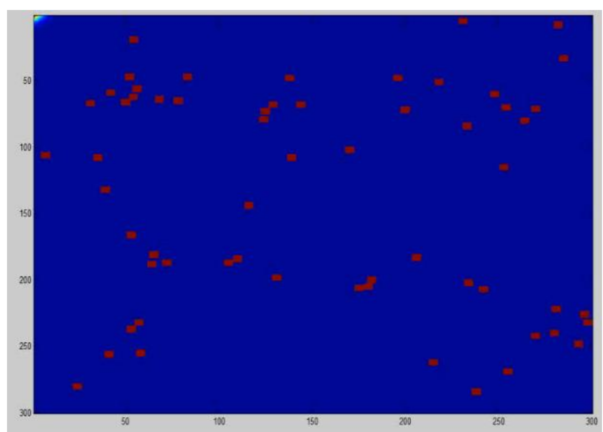


Figure A4



Note: Please view video attached to paper (it will allow the explanation to make more sense)

In the figures presented above, we have five concentrations of a chemical stimulus, which is represented by the areas shaded in dark red. As we go from Figure A1 to Figure A2, we see that the organisms, represented by squares, consume the material quite rapidly. Then, as we go from Figure A2 to Figures A3 and A4, we see that when the organisms finish consuming the material at their respective concentrations, they start to move towards next concentration closest to them. These figures demonstrate how realistic our model is.

As we can see that the even as the material is being eaten it is also continuously diffusing. This leads to an interesting effect, as the material with high concentration of organisms is being devoured when the other concentration which has not been devoured comes in contact or in the range of other organisms that starts getting devoured too. This is an interesting effect that happens due to the diffusion of the material. This enables the organisms to cross over to the point with higher concentration or mathematically speaking with higher gradient. Had there been no diffusion the organisms would have stayed in silo of the concentration they were close to. Diffusion adds another dimension to the study.

3. Gradient Ascent (chemotaxis without diffusion)

Now, the next set of figures shown below demonstrates how each organisms is following the gradient ascent

Figure B1

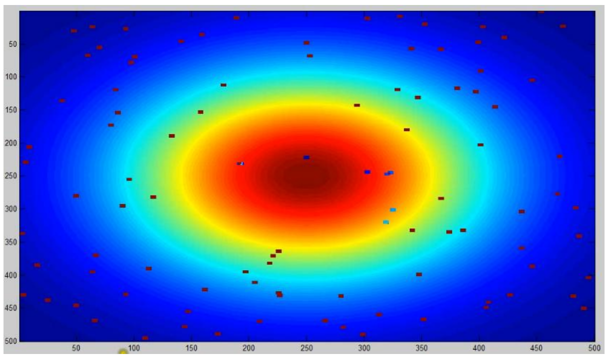


Figure B2

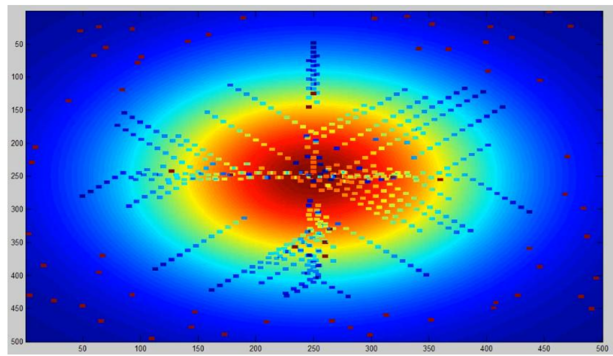
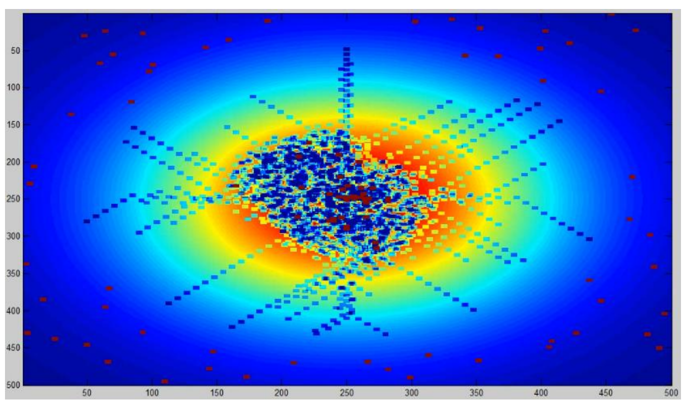


Figure B3



Note: Please view video attached to paper (it will allow the explanation to make more sense)

According to the figures presented above, with only one concentration of a chemical stimulus, we can see that when the organisms are close enough to the chemical stimulus they immediately follow the gradient ascent, with respect to their initial position, towards the chemical stimulus at the center of the graph. We also noticed that the organisms move along their respective gradient ascents quite smoothly, which can be seen in Figures B2 and B3 shown above. The reason why the organisms in the outer regions of our graphs are not moving towards the chemical stimulus and are just remaining idle is because they are too far away to sense the chemical stimulus. Speaking with respect to the code the value of the gradient is too small to have caused a significant ascent to even move one step or move one position in an array. Basically, product of the rate of ascent and the gradient at that point is too small. In reality this can be viewed as it is too far from the concentration to sense it and hence remains at its position.

Also, another interesting observation is the organisms at the center of the concentration field. Note that after a point the organisms that reached the center first also get stuck. This is attributed to the fact that once too many organisms reach a point where the concentration is high and start consuming, they kind of form a well for the organism which is in the center(that is middle of the organisms eating around it). Since, the area around it is devoured it leaves the organism to believe there is no concentration around it and leaves the organism stranded. Again, mathematically speaking the value of the gradient at that point is 0 because there is supposedly a false minima created at that point and the points next to it giving it the illusion of no material left around it.

4. Chemotaxis with noise term

Next, we will be looking into the second case where our model includes the noise term N_t as well as comparing the differences with our model in the first case. Hence, our results for the second case are provided in the figures below.

Figure C1

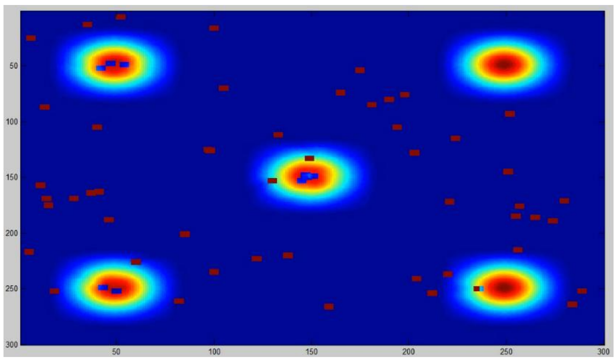


Figure C2

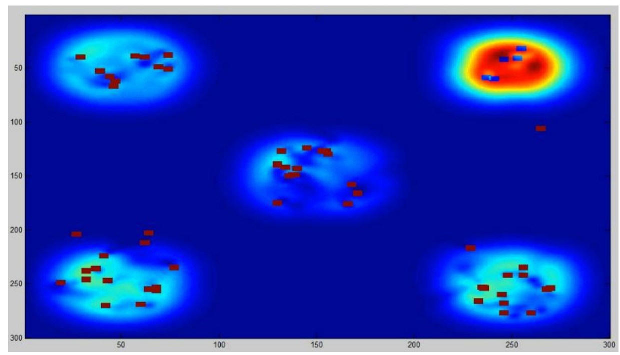


Figure C3

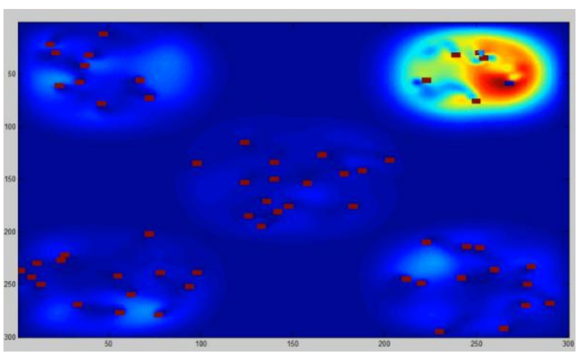
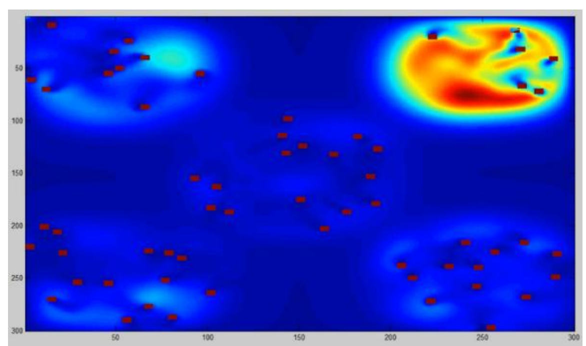


Figure C4



Note: Please view video attached to paper (it will allow the explanation to make more sense)

Again, in these figures, we have five concentrations of a chemical stimulus but the only difference is that this time the movement of the organisms is also characterized by our noise term N_t. From figures C1 to C2, we see that the organisms that are close or within the concentration of the chemical stimulus start consuming the material immediately. However, for the organisms away from the five chemical concentrations, we see that it is taking a little bit of time for them to reach one of the concentrations which is due to the tumbling motion or effect of our noise term N_t. From figures C2 to C3 and C4, we see that when the organisms finish consuming the material at their respective positions, it also takes them a while to move towards the next nearest concentration and a lot them don't even reach the next closest concentration, which is due to N_t.

There are 2 interesting observation here. In the previous case where there was no noise term, the particles were still and had no movement as their movement was contributed solely to the gradient ascent part, now even without being close to the concentration they have a movement which is due to the noise term. Hence, they are in continuous motion.

This leads to the second observation, when they are far from the concentration, that is when the value of the gradient is small their movement is dominated by the random term, but as it reaches close to the concentration due to the noise term the value of the gradient becomes great enough and it runs towards the peak just like it did before. This too translates beautifully into reality in the sense that an organism is continuously in motion looking for higher concentration, when it cannot sense anything it moves randomly but when it starts sensing it starts moving towards the concentration rapidly.

5. Gradient Ascent with noise term

The following figure demonstrates the gradient ascent for our model when we include N_t.

Figure E1

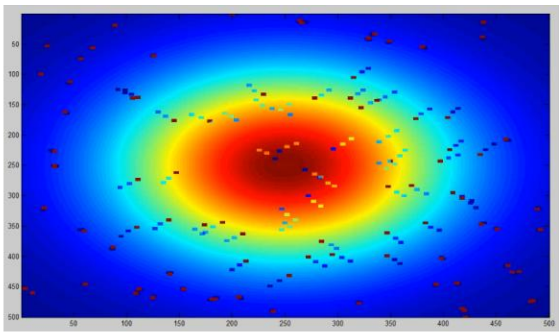


Figure E2

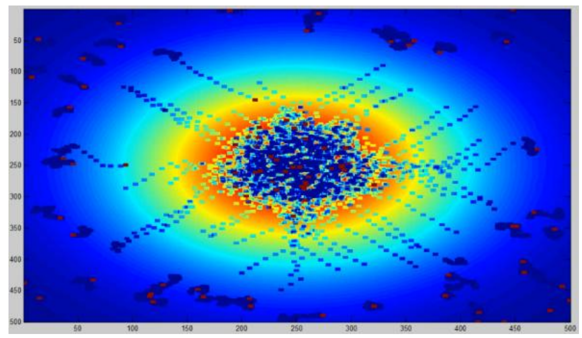
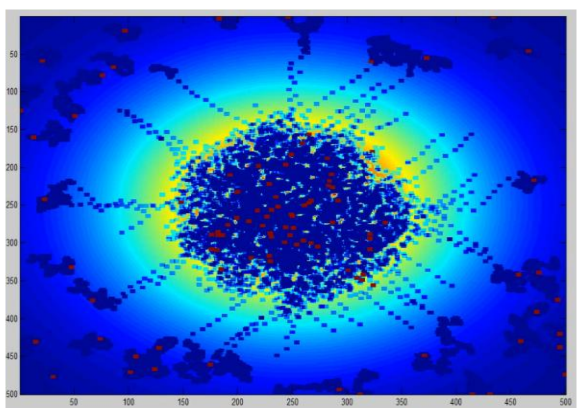


Figure E3



Note: Please view video attached to paper (it will allow the explanation to make more sense)

In figures E1 and E2, we see that the organisms that are close enough to the concentration follow the gradient ascent immediately but in a less smooth and direct fashion when compared to the results for the gradient ascent in the first case, since our organisms are tumbling. However, we also see that the organisms in the outer edges of our graph are continuously moving, due to N_t. Hence, when the organisms are further away from the chemical concentration, we see that their movements are based off N_t, since they are not following the gradient ascent. on the other hand, we see that when such organisms eventually gets close enough to the chemical concentration, there comes a point where the organism's movements is then dominated by the gradient ascent.

This is an interesting example, if we compare the consumption of the material in the case without noise term and with noise term we observe that when the noise is added it consumes more material. This is attributed to the random motion, even though it reaches a point where the value of the gradient is too small it still has a motion and this enables it to reach a point where it might find concentration.

This also solves the problem of the minima caused in the previous case. Even as the element gets stranded to the value of gradient it is always in motion. This enables it to find the material that it wouldn't ideally have found, and once it reaches that point gradient ascent leads it to the places with more possible concentration.

Also, note that there are silos of organisms moving far from the concentration and not reaching the center. Again, this translates into reality as sometimes even with the random motion the organisms never find concentration and keep on moving in their particular region.

6. Implementation

In this section we would like to describe how did we implement following model.

- In order to generate the concentration field we took the function
  f(x,y)=a * e^(-b*(x^2+y^2)). Where a, b are constants. This was to represent a field which increases exponentially as we reach the center and is uniform at a distance from the center.

- The organisms too were created randomly. The function just took the number of bugs to be created and placed them randomly in the field.

- In order to generate the noise term we used the function
  fx=mod(k,5)-2, fy=mod(k,5)-2. Where k=round(100*rand(1))
  As we can see that k would give us any number between 0 to 100 randomly and mod of 5 would give us a number between 0 to 4 and on subtracting 2 we would ultimately get any number between -2 to 2 randomly. We can change the scheme of random numbers as per our choice.

- The core implantation was done in 2 parts and later these 2 parts were merged.
  - Diffusion: We simulated diffusion with different diffusion rates in order to capture the essence of the experiment. A higher diffusion rate caused rapid dissolving of the material and too low caused barely noticing any change.
  - Gradient ascent: As we have said before, we implemented the gradient ascent first. This was done to just understand the movement of organisms without any diffusion.

- Once we implemented these 2 portions we merged them. Of course, we had to make adjustments to the coefficients once we did this.

7. References and links

Links to videos:

- Gradient Ascent:
  http://www.youtube.com/watch?v=TpT4ojuL8v4&feature=youtu.be
- Chemotaxis (without diffusion):
  http://www.youtube.com/watch?v=_pz2Rrh4WoE&feature=youtu.be
- Chemotaxis with noise term:
  http://www.youtube.com/watch?v=fuOiPXrsx4c&feature=youtu.be
- Gradient ascent with noise term:
  http://www.youtube.com/watch?v=4QzzfenxMkY&feature=youtu.be

References:

http://en.goldenmap.com/Chemotaxis
http://www.thefreedictionary.com/chemotaxis
http://en.wikipedia.org/wiki/Chemotaxis#Mathematical_models