Inferring Diffusion from Killed Molecules

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Problem Setup

Inside living cells, millions of molecules are constantly moving. They don't travel in straight lines but instead, their paths look more like random shaking or wandering. We call this type of motion diffusion. Molecules in the cell are affected by the environment, for example, the fluids filling the cell. This environment can eventually cause the molecules to stop moving, an event we call molecules being killed.
The whole process is of interest to biologists, but as one can imagine, modeling the diffusion of molecules in cells is not easy. Even with expensive machines and microscopes, mathematics is still needed to make sense of how these molecules move. The main goal is to understand their diffusion in the cell, ideally using as little information as possible so that complex equipment is not required. The idea is to use the fact that these molecules get killed at some point in time which leads to the central question of this project:

Can we reconstruct the movement of molecules just from the places where they stop?

If we were able to do that, one would only need one frame of the cell, the frame containing the positions of killed molecules, to understand how the molecules diffuse. *Nickl and Seizilles* explained the probabilistic theory behind it and found the general idea of the algorithm. This problem is an inverse problem and Bayesian inference is used to find the solution. Illustration of the forward and inverse problems is shown in Figure 1: the forward problem predicts the killing points of molecules from their trajectories, while the inverse problem reconstructs diffusion from the points where they got killed.

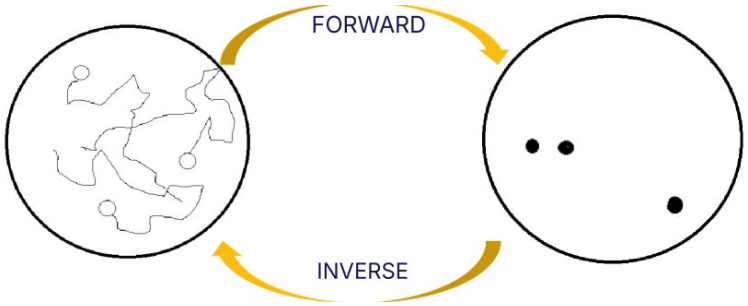

Figure 1: Forward vs. inverse problem in diffusion.

In perfect conditions, one would know exactly when all the molecules were killed, but unfortunately, that rarely happens. It is difficult to determine the precise time when every molecule stops moving, which creates a problem in identifying the frame containing the necessary data - the positions of the killed molecules. The goal of this project was to overcome this obstacle. A similar algorithm was found and experimentally tested. This solution relaxes the assumptions: the required data is just one random frame in time. It is not necessary for all the molecules to be killed, the only data needed at a certain fixed time is the positions of all the molecules, without knowing which ones are still moving and which ones have stopped.
This idea allows us to model the diffusion of molecules using only one snapshot of the situation in the cell. While theory is not as well developed as in the original problem, a lot of experimental work has been done in this relaxed setup, and the results so far are promising.