

## **In silico evolution of chemotaxis**

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Bacteria are able to sense their environment and move towards sources of attractant and away from sources of repellent through the process of chemotaxis. The best understood model for chemotaxis comes from *Escherichia coli*, where the biochemical pathways have been extensively studied. In *E. coli*, the bacterium switches between swimming and tumbling based on the changes in the local concentration of attractant. It is unclear, however, how similar the behaviour and biochemical mechanisms are for other organisms. Work is proceeding on evaluating the chemotactic behaviour of a number of different bacteria, indicating substantial differences with *E. coli*. Even in *E. coli*, the fact that bacteria ‘guttled’ of most of the chemotactic machinery still displays effective chemotaxis indicates that there are still unanswered questions even in this organism. Finally, there are issues about how this particular strategy and implementation have evolved. Was this only one of a number of possible strategies? How did the strategy depend upon the environment, the properties of biochemical networks, or on the evolutionary process? Would similar strategies result under different conditions?

Ideally we would like to take non-chemotactic bacteria and evolve them to perform chemotaxis under a variety of different conditions, a daunting and lengthy experiment. In contrast, we can do this easily in a virtual world. In addition, we can keep complete records of the evolutionary process as it occurs. We create a population of digital organisms that move in a virtual world of attractant. The organisms contain a rudimentary set of biochemical elements, that is, sensors of the external attractant concentration, a reversible motor that can cause the bacteria to tumble or swim, and a set of proteins that can be activated, and while activated, have the potential to activate or deactivate other proteins. We then allow the biochemical network to evolve, selecting those digital bacteria that better co-localise with the attractant to reproduce for the next generation. This allows us to combine molecular-level evolutionary dynamics with phenotype-level selection of a relevant fitness parameter in an exactly specified environment. We find that these digital organisms quickly are able to display effective chemotaxis. Interestingly, the dominant mechanism is one that is very different from that observed in *E. coli*, but is similar to that observed in other bacteria as well as in gutted *E. coli*. The required network can be extremely simple, and can be fulfilled by coupling the bacteria’s metabolic network to the regulatory network, suggesting an explanation for the behaviour of gutted *E. coli* as well as suggesting a possible evolutionary route to how chemotaxis first arose.