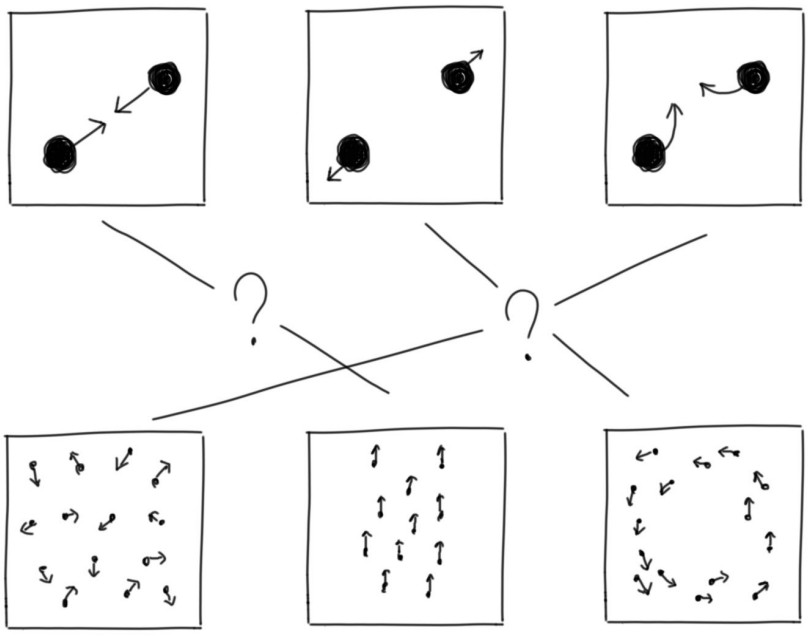
Interactive Evolution of Complex Systems Models

Roujia Wen



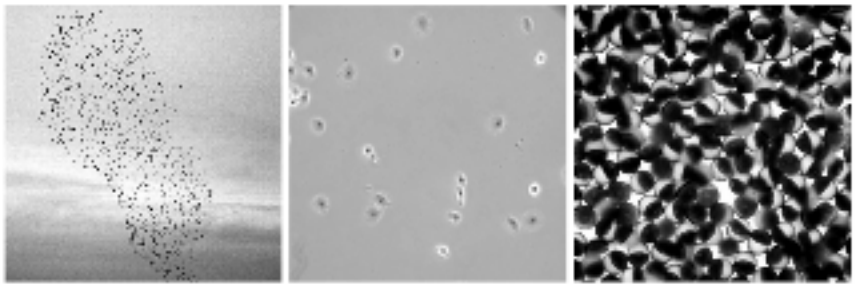
How do microscopic rules of interactions map to global behaviors?

Introduction

This project, in essence, is about how the microscopic rules of interactions in a complex system map to emergent global behaviors. This question is very broad; we can only tackle it little by little, starting with a simple, concrete system. Even though we are very far from fully understanding the psycho-socio-economical factors in higher level complex systems, we do know quite precisely, in a low-level complex system, how physical particles move around when subjected to mechanical and chemical forces. Therefore, in this paper, we focus on one of the simplest models of complex systems—Active Brownian Particles.

What are Active Brownian Particles?

Active Brownian Particles are not an actual class of particles that exist in nature (as are electrons or carbon atoms). They are an abstraction that physicists use to model a wide range of agents that share certain similarities, from nanoparticles, polymers, bacteria, to insects, birds, and robots. These particles are assumed to be disc-shaped[1], identical to one another, and moving on a surface. They are active in the sense that they sustain their motion by some internal propulsion mechanism, as opposed to being passively bounced around (like a bumper car without any power).



Examples of systems that can be modeled by Active Brownian Particles: flocks of birds, motile cells, and synthetic nanoparticles.

We assume that the motion of an Active Brownian Particle is determined by two things: (1) the mechanical forces exerted by other particles, which we can calculate exactly, knowing the positions and momenta of all particles (2) small perturbations from the environment[2], which we cannot calculate exactly, and therefore assume to be a random noise. The term "Brownian," which comes from Brownian motion, refers to the second component.

In other words, the motion of Active Brownian Particles is both stochastic (as opposed to being deterministic) and directed (it's not completely random, but exhibits some order).

[1] Most studies of Active Brownian Particles are concerned with the two-dimensional scenario because of its simplicity. In the three-dimensional case, these particles are assumed to be spherical.

[2] Here when we say "environment", we are referring to everything other than the particles themselves, such as ambient fluids and dusts.

Why do we care? What are some real-world applications?

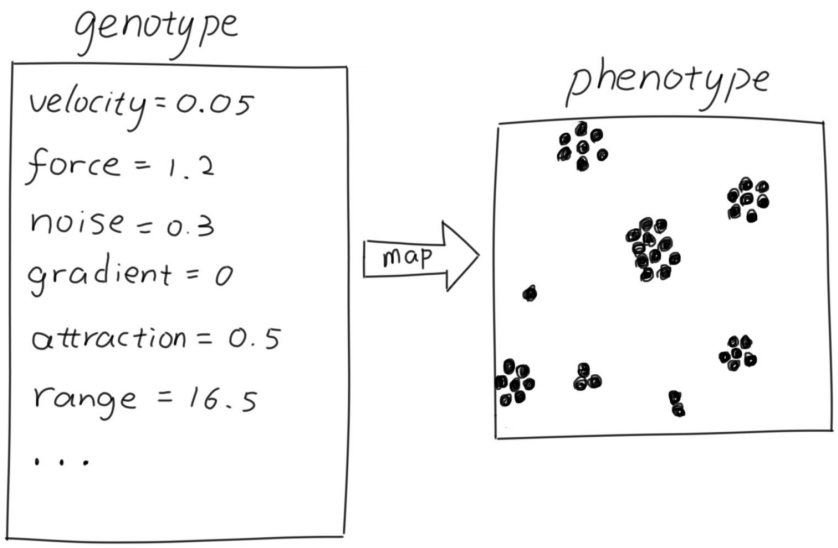
The exact physical mechanisms of interaction among these agents differ from system to system. For example, synthetic nanoparticles realize internal propulsion through induced local thermal or electric gradients; the self-propulsion of enzyme molecules is powered by substrate catalysis; macroscopic animals use chemical energy stored in food to propel themselves. However, when studying Active Brownian Particles, we abstract away the details of the physical mechanisms specific to one system and only talk about concepts like energy, forces, and motion in a context-independent manner. The reason we study such idealized theoretical agents stems from the insight that these systems all share certain similar behaviors at the aggregate level, regardless of their specific physicochemical properties.

The better we understand the mapping between local rules of interactions and the global behaviors of a system, the better we can design agents so that when they interact in aggregate, their collective behavior achieves certain desirable tasks. This knowledge will revolutionize the way we engineer solutions in fields such as biomedical sciences and robotics. Examples of real-world applications include target drug delivery, photothermal therapy, biological toxin removal, environmental monitoring, and water purification. Not to mention the swarms of robotic killer bees in Black Mirror!

A swarm of robotic bees in the television series Black Mirror (S3E6).

The challenges

Using the framework of developmental biology, we can consider the parameter-set of the agents, which encodes microscopic rules of interactions, as the genotype. On the other hand, we view the emergent global behavior or pattern as the phenotype.



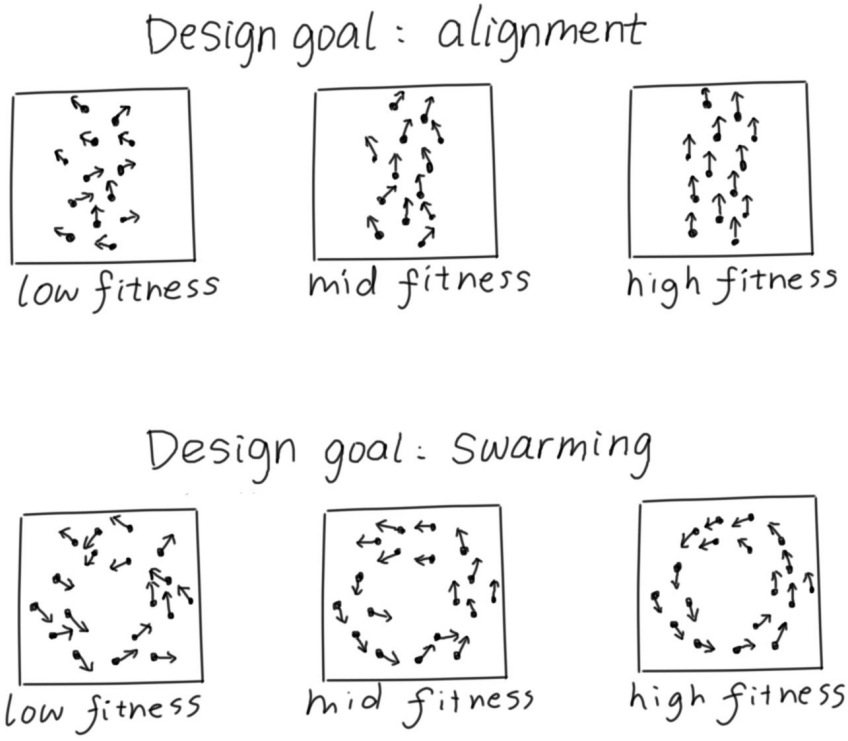
The mapping between the genotype and the phenotype.

This genotype-phenotype mapping is computationally irreducible. In other words, there is no easier way of knowing the emergent pattern of a system than fully simulating the interactions and movements of all particles across a long time span.

Therefore, the problem of finding a genotype that leads to a specific desired phenotype remains a great challenge. Traditional approaches are mostly centered around manual searches, trial and error, and accidental discovery.

A new approach

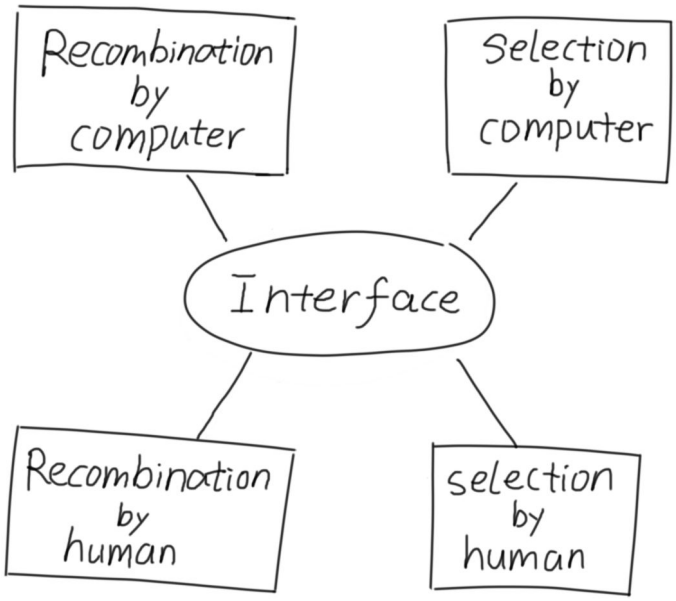
We can frame this problem as an optimization problem: we want to find a genotype with the highest score of fitness—which measures how closely its corresponding phenotype meets the design goal.



Fitness for different phenotypes under different design goals.

The examples above illustrate ways we can quantify fitness. However, in many cases, the fitness which represents desirable characteristics of a spatial structure can be hard to compute or even quantify. Therefore, the usefulness of global optimization methods such as traditional genetic algorithms is limited.

In response to all these challenges, we propose an interactive genetic algorithm which combines human intuition with machine intelligence. The scheme of this approach is illustrated below.



The scheme of the proposed interactive genetic algorithm.

Just like traditional genetic algorithms (TGA), our interactive genetic algorithm (IGA) consists of two iterative steps inspired by natural evolution: recombination and selection[3]. In TGA, both steps are performed by computers. In IGA, on the other hand, a user and a computer collaboratively select for the fittest phenotypes and recombine existing genotypes to create new ones.

In the selection step, two options are available: (1) the user selects desired phenotypes basing on his/her subjective judgment, or (2) the computer selects by calculating and comparing certain statistics that could serve as a measure of fitness.

In the recombination step, there are also two options: (1) the computer recombines genotypes through mutation or crossover, or (2) the user edits the genotype manually.

To further demonstrate the proposed approach, we present a software application with a graphical user interface. You can see how it works and download it from this link:

[3] Traditional genetic algorithms were introduced in Formal Analyses; for a 5-min recap, see https://youtu.be/ejxfTy4ll6I and https://youtu.be/R56DdqdVDi0

https://github.com/roujiawen/soie. A web-based version with minimal functionality can be found at https://roujiawen.com/self-org.

Conclusion

Our solution illustrates a new way to approach the genotype-phenotype mapping problem in systems of Active Brownian Particles by explicitly incorporating human intuition with computational optimization and accelerating the iterations between them. While the computer provides design inspirations through random recombination and evaluation criteria through computable measures, the user provides holistic judgment and inductive reasoning. Moreover, this approach is not limited to systems of Active Brownian Particles; it can be useful for a whole class of similar problems characterized by (1) high-dimensional parameter space (2) irreducible mapping between the parameters (genotype) and the outputs (phenotype), and (3) design objectives that are difficult to quantify or compute.

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