Towards Automated Statistical Physics: Data-driven Modeling of Complex Systems with Deep Learning

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Abstract

Rich phenomena from complex systems have long intrigued researchers, and yet modeling system micro-dynamics and inferring the forms of interaction are challenging for conventional data-driven approaches, being generally established by human scientists. In this study, we propose AgentNet, a generalized data-driven framework to analyze and understand the hidden interactions in complex systems. AgentNet utilizes a graph attention network to model the interaction between individual agents, and employs various encoders and decoders that can be selectively applied to any desired system. Our model successfully captured three different simulated complex systems, namely cellular automata, the Vicsek model, and active Ornstein–Uhlenbeck particles in which, notably, AgentNet’s visualized attention values coincided with the true interaction strength. Demonstration with empirical data from a flock of birds showed that AgentNet prediction could yield the qualitatively same collective phenomena as exhibited by real birds. We expect our framework to open a novel path to investigating complex systems and to provide insight into process-driven modeling.

Keywords Complex systems · Machine learning · Data-driven modeling · Neural network

1 Introduction

Complex systems are collections of interactive agents that exhibit non-trivial collective behavior. The inherent complexity of such systems comes from various points, with interaction range and strength between agents, the exact form of the interaction function, susceptibility to global variables, and the stochastic nature of the decision rule comprehensively affecting the intricacy of analysis. Complex systems are reported in a wide variety of academic fields, from particle spin systems to human societies, and have gathered a significant amount of research interest in the last several decades. In particular, the domain of statistical physics focuses on investigating the micro-level processes that govern emergent behavior in complex systems and modeling them mathematically. Unfortunately, due to the intrinsic complexity of these systems, process-driven modeling to date still strongly relies on human intuition with various prior assumptions and fixed functional forms.

Recently, data-driven modeling (DDM) has emerged as a powerful tool for system analysis alongside the emergence of machine learning (ML) and large-scale data. DDM employs observed data to construct a desired model by optimizing a predefined objective function. Nevertheless, many of the data-driven techniques such as polynomial regression, autoregressive integrated moving average, and Gaussian processes are still restrained by predefined functional forms or kernel functions. Since the functional form of the interactions in a complex system is generally unknown, naive application of such methodology to arbitrary data from a complex system would not yield a proper model.

This has led to deep neural networks (DNNs) attracting great attention from diverse disciplines where the analytic functional form between the input and output is unknown and virtually impossible to express. DNNs are renowned for their performance in optimization and functional expressibility that is practically unconstrained. [1][2] One specialized DNN variant for graph-structured data is the graph neural network (GNN) [3], which models dependencies between
linked agents on a graph and has enabled remarkable progress in graph analysis. An analogy linking relational reasoning and GNN structure was asserted in [4], and this scheme can be similarly applied to complex systems. One may depict a complex system as a dynamically changing graph in which each vertex is an agent and links between agents indicate interaction. In this approach, the problem of modeling the micro-dynamics of single agents becomes equivalent to properly inferring the effect from other agents on a graph and estimating the state transition of each individual agent at the next time step.

Inspired by these recent attempts, we introduce AgentNet, a generalized neural network framework based on graph attention networks (GATs) [5] to model single agents in complex systems. AgentNet approximates the transition function of the states of individual agents by training the neural network to predict future state variables. Our model jointly learns the interacting range, strength, and overall function from observed data in an end-to-end manner with minimum prior assumptions about the system. We applied AgentNet to complex systems with more than 1800 agents, greatly exceeding previous ranges [4, 6, 7] of at most several dozens of agents. Furthermore, visualization of the inner modules as granted by our framework enables a clear interpretation of the trained model, which also provides insights for process-driven modeling. The capability of AgentNet is demonstrated here via data from simulated complex systems: cellular automata [8], the Vicsek model [9], and the active Ornstein–Uhlenbeck particle [10] model, along with application to real-world data comprising trajectories in a flock of birds [11].

2 Related works

2.1 Data-driven modeling

Data-driven modeling, an umbrella term for numerous techniques, generally refers to a methodology that finds a relationship between state variables or their time evolution from observed data [12]. This is the exact opposite approach from that in conventional statistical physics, which starts from a microscopic description of interacting agents and then derives observables. Hence, DDM shares the same spirit as inverse problems [13, 14], and is also closely related to diverse disciplines of statistical inference such as ML, data mining, and automated science [15, 16].

DDM usually employs a small amount of explicit knowledge of the system, though there should be some prior assumptions underlying the method itself. For instance, the outcome of the generalized linear model is assumed to be generated from a distribution from the exponential family, an approach which cannot be applied to approximate distributions having multiple modes or consisting of mixed models. As one of the most prominent models in DDM,
DNNs are relatively free from the constraint of assumptions due to their remarkable expressive power. It has been shown that DNNs can approximate virtually any arbitrary continuous function, even with only a single hidden layer of sufficient width [1].

From this outstanding functional expressiveness, applications of DDM to the analysis of complex systems have naturally appeared. Some of the early works demonstrated the predictive power of DNNs by employing a complex system as a testbed [17, 18], while others showed the potential of DNNs as knowledge extraction tools for complex systems and collective behavior [19, 20, 21]. In recent decades, neural networks have been applied to various complex systems in both statistical physics and ML, in such works as learning differential equations from observed data [22, 23, 24], unveiling physical concepts in an unsupervised manner [25, 26, 27], and reconstructing quantum states in many-body quantum systems [28]. In particular, pedestrian dynamics has received significant attention from ML researchers in tandem with the increasing popularity of self-driving vehicles; multiple neural architectures dedicated to predicting the future trajectories of moving agents have been proposed [29, 30, 31, 32], which have influenced the model developed in this paper.

2.2 Graph attention network

Graph neural networks include various models that receive graphs as inputs and perform computations on the vertices and edges to accomplish a certain task. From the early era of GNNs, predicting the state of interacting agents has been widely selected to verify model performance [5, 6, 7]. Explicit correspondence of formulation between a GNN and a system of interacting agents was underlined in a work introducing the Interaction Network [4], with a thorough review of this correspondence provided in [3]. While other literature has covered analogous concepts [34, 35, 36] by modeling complex interaction between agents with GNNs, applications of most studies to date lack a visibility of the interaction strength or are restrained to systems with limited characteristics and small numbers of agents.

The GAT introduced in [5] combined a GNN with an attention mechanism [37] that explicitly assigns normalized weights to the importance of information $\alpha_{ij}$ by

$$\alpha_{ij} = \frac{\exp(e_{ij})}{\sum_{k \in R_i} \exp(e_{ik})},$$

where $e_{ij}$ is the attention coefficient between agents $i$ and $j$, and $R_i$ denotes the set of agents that is linked to the $i$th agent on a graph. Attention coefficients are calculated by a specific attention mechanism and function as a weight that is multiplied to the information from the $j$th agent while considering the state transition of the $i$th agent.

One of the advantages of this approach is that we can indirectly analyze the interaction strength between agents on the graph. Many prior works have regarded attention weight ($\alpha_{ij}$) as a proxy for interaction strength [20, 31, 32]—our study is the first in-depth demonstration of this assumption, achieved by comparing the attention weight to the groundtruth interaction strength in simulated complex systems. Our framework, AgentNet, is constructed by setting a modified GAT as the core module and adopting multiple encoders and decoders that can be selectively applied for given system characteristics or desired output.

3 Notation and Concepts

3.1 Types of Complex Systems

From cellular automata to human societies, complex systems have diverse characteristics that are difficult to incorporate into a single modeling framework. By virtue of the flexibility of modern neural networks, one can modify specific elements of a particular network structure to fit system characteristics while maintaining the core of the network. In this way, AgentNet addresses a variety of system characteristics as follows.

- **Continuity:** The state variable of an agent can have either discrete, continuous, or even a mixed set of values, and neural networks can freely handle all these input types since they receive a vector of rational numbers. The output of neural networks can also be discrete, continuous, or mixed. For the case of a discrete and bounded number of output, we can regard each output as a class and let the neural network minimize the cross entropy; otherwise, we can regard the problem as a regression problem and minimize the mean squared error.

- **Stochasticity:** The decision rule of a complex system can be either deterministic or stochastic. While a simple neural network is by nature deterministic, there are several ways to construct a neural network with probabilistic output [38, 39, 40, 41]. In this study, we employ a Gaussian neural network as the decoder of the stochastic AgentNet, which produces means and a covariance matrix of multivariate Gaussian distribution.
We assume that the system has at most pairwise interaction without any higher-order interactions. This assumption can be alleviated by employing a GNN with a hypergraph structure that considers hyperlinks as a direct extension of 42. The main reason to introduce self-interaction, and $h_{ij}(s^t_i)$ captures the pairwise interaction between the $i$th and $j$th agents. The interacting function $h_j$ can be expanded further by factoring out the interaction strength $h_{R_i}$, which is subject to the neighbor set of the $i$th agent, $R_i$, defined as

$$R_i = \{a_j \in A \mid a_i \text{ interacts with } a_j\}. \tag{3}$$

The main reason to introduce $R_i$ and $h_{R_i}$ is to explicitly express interaction range and strength; the significance of this will be explained in later sections.

With $h_{R_i}$, the interaction function $h_j(s^t_i)$ expands as follows,

$$h_j(s^t_i) = h(v^t_{ij}, h_{R_i}(v^t_{ij})), \tag{4}$$

where the set of variables $v^t_{ij} = \{s^t_i, s^t_j, U^t\}$ denotes two state variables along with global variables. Our formulations of agent-based complex systems are shown in Fig. 1A. Table S1 in the SI Appendix shows the functional form of each model system according to our formulation.

### 3.2 Problem definition

In this paper, we mainly focus on a system consisting of $N$ agents for which the state of each agent until time $T$ is (at least partially) identified and observed. Here, the state of the variables differ by system and may not be unique. For instance, both (1) position and velocity at the current time step and (2) several steps of position trajectory with a sufficiently small time step can deliver approximately the same amount of information. Note that in real scenarios, it is safe to include every observed variable as a state variable since we generally do not have prior knowledge of variable importance, and moreover, the neural network may effectively filter out irrelevant variables in its decision.

We denote the set of all agents as $A = \{a_1, a_2, \ldots, a_N\}$ and the corresponding observed state variables of all agents at time $t$ as $s^t = \{s^t_1, s^t_2, \ldots, s^t_N\}$. In addition, the system might have time-dependent global variables $U^t$ that affect agent interaction, such as temperature in a thermodynamic system. For simplicity, we derive our formulation in a Markovian setting, where the state variable $s^{t+1}$ solely depends on $s^t$ and $U^t$. We note that a similar logic also applies to non-Markovian systems.

Agent modeling aims to identify the transition function of individual agents, which can be written as $s^{t+1} = f_i(s^t, U^t)$. We assume that the system has at most pairwise interaction without any higher-order interactions. This assumption can be alleviated by employing a GNN with a hypergraph structure that considers hyperlinks as a direct extension of the current study. The general form of the transition function $f_i(s^t, U^t)$ can be expressed as

$$f_i(s^t, U^t) = f(h_1(s^t_i, U^t), \ldots, h_{i-1}(s^t_i, U^t), g(s^t_i, U^t), h_{i+1}(s^t_i, U^t), \ldots, h_N(s^t_i, U^t), U^t), \tag{2}$$

where $g$ denotes self-interaction, and $h_j(s^t_i)$ captures the pairwise interaction between the $i$th and $j$th agents. The interacting function $h_j$ can be expanded further by factoring out the interaction strength $h_{R_j}$, which is subject to the neighbor set of the $j$th agent, $R_j$, defined as

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Figure 2: Result of AgentNet for cellular automata. (A) Attention weight transition of a single target cell throughout the training. In the initial stage, the model has no information about interaction range and assigns nearly similar values to all of the cells in the system. Attention gets narrowed down to a smaller region as training advances, and finally concentrates into eight surrounding cells, which is the theoretical interaction range. (B), (C) AgentNet predictions with respect to given alive and dead microstates, respectively. The total number of alive cells in the neighborhood is denoted by $s$, which is the sole parameter of the CA decision rule.

In most cases, the exact analytic forms of $R_i$, $h_{Ri}$, $h_j$, and overall function $f$ are completely unknown, and it is infeasible to elicit these functions from observed data alone. Especially, blindness to interaction strength function $h_{Ri}$ significantly complicates this inverse problem since we have to test every possible combination of neighbor candidates while simultaneously guessing the correct nonlinear functional form of $h_j$. The problem becomes harder if the states are correlated in time since this expands the range of possibly correlated variable pairs further out in the time dimension. To sum up, many of the current methodologies are not capable of DDM for complex systems without strong prior assumptions regarding the functional form.

4 Model description

4.1 AgentNet

AgentNet is a generalized framework for the data-driven modeling of agent-based complex systems, influenced by previous works and reinforced with several modifications. The base module of AgentNet is similar to a GAT with transformer architecture [37], where each agent decides its next state by putting information from itself and the attention-weighted sum of other agents together. AgentNet initially operates on a fully-connected graph, implying that it initially assumes every agent as a possible neighbor and gradually learns the true interaction strength by training. Our model first encodes the state variables of agent $s^t$ with an encoder, then passes the information to the transformer which computes the impact from the entire system state $s^t$, and finally decodes the outcome with a decoder. AgentNet has various options for its encoder and decoder depending on system characteristics and desired outcomes. More detailed architectures and implementations are described in the SI Appendix.

Our formulation of an agent-based complex system coincides with concepts in the GAT core, as depicted in Fig. 1B: self-loop calculation captures the self-interaction $g$, attention weight with others captures the interaction strength $h_j$, and the weighted sum along with the decoder corresponds to overall function $f$. Particularly, interaction strength can be easily identified by visualizing attention weight. Despite the fact that neural networks are infamous for being black-boxes, natural correspondence between an agent-based complex system and the formulation of a GAT enables us to further investigate the approximated function individually, thereby turning AgentNet into a gray-box [43].
One major difference between AgentNet and prior models is in the calculation of attention weight. The most commonly used attention mechanisms are additive attention, \cite{44} where information from agents is added to each other, and multiplicative attention \cite{45}, which employs inner products. We have found that neither mechanism is suitable for the aim of AgentNet, as verified by their low performances. Unlike previous applications of attention mechanisms for sequential information, interaction strength in a complex system can be highly nonlinear and asymmetric. Thus, we employ separate multiple perceptron layers to calculate attention instead of a single perceptron layer as in additive attention. This \textit{neural attention} enables much more flexible representations of attention. Although it increases the number of parameters and overall training cost, we have observed that neural attention shows qualitatively superior performance as compared to additive and multiplicative mechanisms in tasks for AgentNet. Detailed verifications and results can be found in SI Appendix.

Another modification of AgentNet arises from the dynamic nature of complex systems and their observation. In graph theory, a dynamic graph refers to a graph in which vertices or links may change over time. Some complex systems with an exchange of agents are dynamic in nature, but even in a non-dynamic system, observed data could take the form of a dynamic graph. For instance, observation data from an animal flock usually contains a number of trajectories that all start and end at different times, effectively yielding a dynamic interaction graph. Limitations of time, observation angle, and resolution lead to imperfect and split trajectories of agents that cannot be handled by conventional recurrent neural networks or GNNs. Many previous works evaded this problem by only considering agents with full-time trajectories \cite{29,30}, ignoring the other agents that might affect the decision rule. Likewise, while several previous approaches could handle graphs with dynamic edges \cite{46,47,48}, none of them could process graphs with dynamic nodes.

To the best of our knowledge AgentNet is the first attempt to deal with dynamic nodes on a spatiotemporal graph. We employed a specialized LSTM encoder for a dynamic graph that checks the status of each agent. At every time step \(t\), AgentNet inspects whether the trajectory data of each agent was recorded at times \(t\) and \(t-1\). Every agent that has existed from \(t-1\) inherits the previous LSTM cell’s hidden states, otherwise it creates a new LSTM cell initialized by another trained multi-layer perceptron. Also, agents that do not exist at time \(t\) are excluded in the attention calculation by setting their attention to zero, which is equivalent to cutting the link to non-existing agents on the interaction graph at time \(t\). With the aid of these inspection schemes, we can exploit maximum information from the temporally disjointed and spatially connected time series without any discarded datapoints.

5 Experiments

We implemented our AgentNet model with PyTorch \cite{49}, and all of the neural network models consist of comparable numbers of parameters. More detailed descriptions and implementations can be found in the SI Appendix.

5.1 Cellular Automata

In the CA model, each cell has its own discrete state, either \textit{alive} or \textit{dead}. Each cell interacts with eight adjacent neighbors, and the state of each cell evolves according to the following rules.

- A live cell stays alive if two or three neighbor cells are alive. Otherwise, it dies.
- A dead cell becomes alive if exactly three neighbor cells are alive. Otherwise, it remains dead.

We simulated 1,000 sets of data and label pairs to train the AgentNet for CA. In each pair, the data is a 14 \times 14 grid of cells with initially randomized states, and the label is the state of the grid after a single time step. Since the cells at the corners and edges have no proper neighborhood, we discarded these cells and therefore only the inner 12 \times 12 grid was updated and used for training.

From the perspective of AgentNet, CA is a binary classification problem, i.e. whether each cell becomes alive or dead at the next time step. AgentNet for CA receives three state variables: positions \(x^t\) and \(y^t\), and cell state \(c^t\). The output here is a list of expected probabilities that each cell becomes alive. We use the binary cross entropy loss function between the AgentNet output and the groundtruth label as

\[
L_{BCE}(s) = \sum_i y_i \log c_i + (1 - y_i) \log (1 - c_i),
\]

where \(c_i\) is the predicted \(i\)th cell state of output \(s\), and \(y_i\) is the corresponding true label of the \(i\)th cell.

Figure 2 summarizes the results of AgentNet for CA. Figure 2A depicts the attention weight \(w\) of the target cell (in this case, the 115th cell) across the entire grid. After 70 epochs, AgentNet quickly \textit{realized} that a vast majority of the cells are irrelevant to the target cell and thereafter concentrated its attention to a more compact region. AgentNet figured out
Figure 3: Result of AgentNet for the Vicsek model. (A) Attention weight visualization of two sample cells, \(a_1\) and \(a_2\). Both cases show a circular sector of attention distribution with clear boundaries. (B) AgentNet position predictions for the two sample cells \(a_1\) and \(a_2\). Circles indicate the starting positions of the two particles, with the two heatmaps showing the AgentNet prediction along with the means of predicted distributions (Xs). The model predicts the expected theoretical distribution (crosses) with great precision, even when the given training samples (green and blue stars) are distant from the means of the theoretical distribution.

The true interaction range after 150 epochs, although it took another 100 epochs to perfectly employ the information it gathered to decide the next cell state.

Figure 2B and 2C show the output of AgentNet after 250 epochs of training. As the decision rule of the CA model is only affected by a microstate of \(3 \times 3\) grid cells with the target cell in the middle, all of the other cells are irrelevant. Thus, we can investigate the micro-dynamics of the trained model by verifying all possible \(2^9 = 512\) microstates located in a randomly distributed environment. In Fig. 2B and 2C, each microstate was tested in 1000 different environments, and AgentNet showed an exact match to groundtruth labels in both cases of alive and dead target cells. This demonstrates that AgentNet can jointly infer the interaction range and decision rule of a single agent in a discrete Markovian system.

5.2 Vicsek model

The concept of active matter was first introduced to describe a system in which a large number of agents consume energy and exert intrinsic force. The rich phenomenology of active matter systems such as collective motion has motivated researchers in a wide range of disciplines.\[50, 51, 52\] One of the earliest and most prominent models to describe an active matter system is the Vicsek model\[9\], where each agent averages the velocity of nearby agents (including itself) to replace its previous velocity. At each time step, every agent updates its position by adding this newly assigned velocity with stochastic noise. The exact formulation of the VM model is described in SI appendix, Table S1.

Since the decision rule in this case is stochastic, we employed a probabilistic version of AgentNet for predicting the position distribution of the next time step. AgentNet for VM receives four state variables, positions \(x^t\) and \(y^t\), and velocities \(v_x^t\) and \(v_y^t\), and predicts the positions of the next time step \(x^{t+1}\) and \(y^{t+1}\). More precisely, the model infers the parameters of a two-dimensional (2D) Gaussian distribution, mean vector \(\mu = (\mu_x, \mu_y)\), and \(2 \times 2\) covariance matrix \(\Sigma\). We used the negative log likelihood (NLL) loss function for multivariate Gaussian distribution to train the AgentNet for VM as

\[
L_{NLL}(s) = \sum_i -\frac{1}{2} \log(\det(\Sigma_i)) - \frac{1}{2}(y_i - \mu_i)^T \Sigma^{-1}(y_i - \mu_i),
\]
Figure 4: Results of AgentNet for AOUP. (A) In both panels, eight steps of training data of four particles are drawn with black dots, starting from the large black dots. AgentNet predictions of the trajectories in the following 12 steps (right) perfectly coincide with the sample trajectories from the true Langevin equation (left). 100 samples are drawn in both panels, and the final positions are highlighted with white stars. (B) Equilibrium state of a system with $R = 5$, which is unseen at training time. A single realization from the true distribution is drawn with final positions marked by red stars (left), while a single sample from the predicted distribution of AgentNet is drawn with final positions marked by blue stars (right). AgentNet for AOUP captures the generalized effect of interaction length $R$ and predicts the collective behavior of the untrained system. (C) Exerted force on and attention assigned to particles shows great coincidence under a linear fit of $c = 2.1$ and $b = -0.02$. Scaled attention $\alpha_{ij}$ and exerted force $F_{ij}$ are collected from the AOUP system with $R = 4$. Attention visualization for a single target particle (blue) is depicted in the inset.

where $\mu_i$ and $\Sigma_i$ are the output of the $i$th agent, and $y_i$ is the corresponding label of the $i$th cell. Note that $y_i$ is a single stochastically sampled value, thus putting AgentNet for VM in the difficult condition of trying to identify the decision rule with only one sample for each environment.

As a result, AgentNet for VM achieved an NLL loss of $-0.856$, while the theoretically computed NLL loss was $-1.301$. We note that other approaches such as naive multi-layer perceptrons failed to achieve meaningful prediction and resulted in an NLL loss of around $+1.0$. Figure 3A visualizes the attention weights of two sample agents, $a_1$ and $a_2$. AgentNet for VM accurately learned the interaction boundary of the given VM, which resembles a major sector of the circle, after 200 epochs of training. The predicted position distributions for these two sample agents are depicted in Fig. 3B. We observe that AgentNet precisely estimated the groundtruth distribution with true mean, even though the given training data was sampled from a stochastic distribution and did not match the expected mean value. This shows the capability of AgentNet to learn the general transition rule governing the entire set, rather than merely memorizing every single training datapoint and overfitting to them. We report that AgentNet shows the same outcome with unseen test data.

5.3 Active Ornstein–Uhlenbeck Particle

Differing from the Vicsek model, some active matter shows a time-correlation of particle positions due to the force inherent in the particles that allows them to move. These systems are generally referred to as self-propelled particles, which can be described by overdamped Langevin equations for the position $x_i$ of each particle as

$$
\gamma \dot{x}_i = F_{i}^{ext} + F_{i}^{int} + \sqrt{2\gamma T} \eta_i + \gamma f_i,
$$

where $\gamma$ is the drag coefficient and $T$ is temperature. Here, $F_{i}^{ext}$ is the external potential, and $F_{i}^{int} = -\nabla_i V$ is the total force exerted on particle $i$ due to the soft-core potential from other particles, $V = \exp(-|r_{ij}|^3/R^3)$, that depends on relative distance $r_{ij}$ and interaction length $R$. This internal potential is the so-called generalized exponential model of exponent 3 (GEM-3) potential. In this study, we use AOUPs confined in a harmonic potential as an example system,
describing the intrinsic propulsion force $f_i$ as an independent Ornstein–Uhlenbeck process as

$$\tau f_i = -f_i + \sqrt{2D_f}w_i$$

(8)

where $\tau$ is correlation time, $D_f$ is a diffusion constant, and $w_i$ is a standard Gaussian white noise. As an external potential, we apply a weak harmonic potential $F^{ext} = -kx_i$ with spring constant $k = 0.1$ to confine the particles, as broadly assumed and experimentally employed \([53]\).

The AOUP model with GEM potential shows roughly hexagonal clusters of particles, with stronger diffusion constant $D_f$ weakening its regularity and resulting in a noisy cluster core. \([10]\) The periodicity of the hexagonal pattern is known to be approximately $1.4R$ with no $F^{ext}$ \([54]\); different interaction length $R$ then yields different patterns and therefore different dynamics. In this study, we trained AgentNet for AOUP with the data from a system with various interaction lengths $R$ to demonstrate how AgentNet handles changes of global variables. We attached a constant vector of $R$ to the encoder and the attention vector to open the possibility that both overall function and interaction function $h_{R_t}$ separately depend on $R$. (In case of AOUPs, it only affects $h_{R_t}$, since $R$ only affects interaction potential $F^{int}$.)

AgentNet for AOUP adopted an LSTM model as an encoder to enable iterative data generation. The model observes 8 steps of trajectories as input data and the loss is calculated for the next 12 steps with respect to the labels. Exact details of the constants and step size used to generate training and test data are described in SI Appendix. We simulated 8000 sets of training data and label pairs of 100 particles, consisting of four state variables, $x^a, y^a, v_{x}^{a,t}$, and $v_{y}^{a,t}$, and a global variable $R$ ranging from 2.0 to 4.0. The model predicts parameters for a 2D Gaussian distribution as similar to the AgentNet for VM case, and uses the same NLL loss as described in \([6]\) Differing from the VM case, AgentNet for AOUP yields two separate sets of parameters for positions $x^{a,t+1}$ and $y^{a,t+1}$ and velocities $v_{x}^{a,t+1}$ and $v_{y}^{a,t+1}$. This is necessary because input and output state variables should be the same in order to iteratively sample from the predicted distribution and feed it into the prediction at the next step. Note that the internal variable, $f_i$, which has its own Ornstein–Uhlenbeck dynamics, does not present in the input data and thus the neural network has to infer this hidden variable by eight steps of past trajectory. Also, we found that in the case of AOUP, predicting the difference of the particle states instead of directly predicting the states themselves is numerically stable and accelerates the training time.

First, we compare the average displacement error (ADE) and final displacement error (FDE) of our model among 12 predicted steps as in previous works \([30,29]\) along with a linear extrapolation and naive LSTM without the graph attention core as baselines. AgentNet for AOUP showed ADE/FDE of 0.0381/0.0548, while linear extrapolation and naive LSTM showed much lower performances of 0.210/0.465 and 0.158/0.316, respectively. Figure 4 summarizes the qualitative result of AgentNet for AOUP. In Fig. 4A, 100 trajectories sampled from the ground truth Langevin equation and Agentnet for AOUP are depicted. Our model precisely predicted the future trajectories subject to the past states. The effect of the global variable $R$ was also properly captured, as shown in Fig. 4B. The model prediction shows a hexagonal pattern of periodicity $\tau$, which coincides with the theoretical value of periodicity when $R = 5$. This verifies a capability of generalization since the model had never been trained on the condition of $R = 5$ and yet still properly captured the collective phenomena. Finally, we demonstrate that the attention $\alpha_{ij}$ that target particle $i$ assigns to another particle $j$ corresponds to the theoretical force $F_{ij}$ that particle $i$ exerts on particle $j$, up to linear fitting. In Fig. 4C, we draw the scaled attentions and exerted forces $F_{ij} = \nabla V_{ij} = (-3\beta_i^2 \exp[-r_{ij}^3/R^3]) / R^3$ versus the relative distance to the target particle $r_{ij}$. In spite of a slight disagreement at small $r_{ij}$, scaled attention well matched $F_{ij}$ and therefore can be considered as a proxy for interaction strength. AgentNet for AOUP successfully predicted and investigated one of the most complex systems possessing internal potential, external potential, memory effects, and stochastic noises.

### 5.4 Chimney swift trajectory

Finally, we demonstrate the capability of our framework through predicting the empirical trajectories of a freely behaving flock of chimney swifts (CSs). Bird flocks are renowned for their rich diversity of flocking dynamics, for which models with various mechanisms such as velocity alignment and cohesion have been proposed in the last several decades \([9,55,56]\). We employed a portion of the data from \([57]\), recorded in Raleigh, North Carolina in 2014. The flock data contains 30 min of observed CS trajectories at 30 frames (s) per second, with approximately 100,000 unique trajectories and a maximum of 1848 birds at one instance. The reason that the number of unique trajectories greatly exceeds the size of the flock is because many of the trajectories from the same birds are separated if (1) they escape from the sight of the cameras and re-enter after, and (2) the birds are occluded by other birds thus introducing ambiguity. Since half of the trajectories last less than 150s = 5s and 80% last less than 300s = 10s, discarding non-full trajectories as previous works would significantly reduce the number of birds to consider at a given time step. To handle these disjointed yet entangled pieces of trajectories, we inspected the data at every step of the LSTM to manually connect the hidden states from the past, exclude the nonexistent birds at a certain time, and start a new chain of hidden states from a separate neural network if an agent newly enters the scene.
Figure 5 summarizes the results of AgentNet for CS. The predictive power of AgentNet is illustrated in Fig. 5A, where linear extrapolation and naive LSTM show almost similar results while AgentNet shows greatly reduced errors at predicting longer time steps. Figure 5B, showing the visualized attention of a typical bird, clearly indicates the near-sighted and forward-oriented nature of the bird’s interaction range. To verify this interaction range, we averaged the attention values from the first step of predictions according to the relative coordinates of the target bird. The averaged results from the first 10 sets of test data are drawn in Fig. 5C. The interaction range of the sector form coincides with previous literature about biological agents’ visual frustum, which depends on forward-oriented sight and relative distance from each agent. [11, 20, 56, 58] We have observed that the angular concentration of averaged attention changes by time, but the interacting range remains around 15 to 20 m. Further discussion on the attention heatmap is described in SI. appendix.

Finally, we reveal the capability of modeling collective behavior by comparing naive LSTM and AgentNet for simulation data over longer times. As seen in Fig. 5D, the naive LSTM could not capture the collective movements of the flock and simply modeled the birds to fly in the same direction with no cohesion. In contrast, Fig. 5E shows a collective movement in which all birds are gathered into one giant flock that exhibits complex flocking shapes, which is not present in the training data, thereby properly modeling collective behavior. This claim is further supported by Fig. 5F,
Table 2: Models to test the performance of AgentNet and their respective characteristics.

| System                              | Continuity | Stochasticity | Memory effect | Empirical data |
|-------------------------------------|------------|---------------|---------------|----------------|
| Cellular automata                   |           |               |               |                |
| Vicsek model                        | ✓          | ✓             | ✓             |                |
| Active Ornstein–Uhlenbeck particle  | ✓          | ✓             | ✓             |                |
| Chimney swift flock                 | ✓          | ✓             | ✓             |                |

The X’s indicate the opposite characteristics: discrete, deterministic, Markovian, and simulated data, respectively.

which plots similar qualitative behaviors of angular momentum and mean dispersion from centroid in both real data and AgentNet simulation, but not in the naive LSTM case that reflects repetitive and linear motions without any flocking.

6 Conclusion

This study proposed AgentNet, a generalized framework for the data-driven modeling of a complex system. We demonstrated the flexibility, capability, and interpretability of our framework with large-scale data from various complex systems. Our framework is applicable for practically any agent-based system as long as the system is governed by at most pairwise interaction, and a sufficient number of observation data is available. In addition to yielding an outstanding prediction model for a single agent, the proposed framework can infer and visualize interaction strength between agents, which could assist researchers in gaining clearer insight into given systems and their dynamics. Furthermore, AgentNet is scalable for an arbitrary number of agents due to the nature of GNNs, thus facilitating free-form simulation of the desired system with any initial condition.

There are several domains in which AgentNet is anticipated to exhibit its full potential. As we demonstrated via AOUP and CS, the analysis of active matter such as bacterial cells [53, 59] or pedestrian prediction [29, 30] may benefit from this approach. One interesting application we are looking at is connecting AgentNet to network analysis. While we focused here on systems without known interaction ranges, GNNs were originally proposed for data with graph structures. By incorporating an adjacency matrix instead of assuming a complete graph, AgentNet may yield data-driven models of both agents on a network or nodes of a network. Typical application examples would be the analysis of network dynamics [60] such as information propagation through networks including epidemics [61] or rumor spreading [62].

We could further apply different encoders and decoders to improve the performance and include available domain knowledge. For instance, a decoder with a single Gaussian distribution may not be suitable to approximate multimodal or highly irregular distributions. In such cases, a different decoder may produce more flexible output, such as a Gaussian mixture model, [40] or even be substituted by a variational model [30] that could approximate an arbitrary distribution. Also, as mentioned earlier, the hypergraph neural network [42] could facilitate the analysis of a system with higher-order interactions. We highlight the virtually unbounded scope of the proposed framework in this study, and hope that AgentNet shines a new light on agent-based modeling and helps researchers in diverse domains reach into their systems in a data-driven manner.

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8 Supporting Informations

1. Dataset details

Cellular Automata

We employed Cellular Automata (CA) model based on the rule of Conway’s life game [8]. As described in experiments section in the main manuscript, CA takes place on regular grids and each cell on the grid alters its cell state in each time step according to specific set of rules. The rule of life game is often notated as B3/S23, which means dead cell regenerates with 3 neighbor live cells, while live cell stays alive with 2 or 3 neighbor live cells. In this study, we used
Table 3: System formulation of model systems for demonstration.

| System               | Cellular Automata                                                                 | Vicsek model                                                                                        | Active Ornstein-Uhlenbeck Particle                                                                 |
|----------------------|-----------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------|----------------------------------------------------------------------------------------------------|
| $s^i_t$              | $\{x^i_t, y^i_t, c^i_t\}$                                                        | $\{x^i_t, y^i_t, v^e_x, v^e_y, v^i_t\}$                                                            | $\{x^i_t, y^i_t\}$                                                                                 |
| $a^i$                | None                                                                              | None                                                                                                | $R$                                                                                                |
| $R_i$                | $\{a_j \in A | (x^i_t - x^j_t) + (y^i_t - y^j_t) \leq 2\}$                           | $\{a_j \in A | r(s^i_t, s^j_t) < r_c, |\theta(s^i_t, s^j_t)| < \theta_c\}$                       | $A - \{a_i\}$                                                                                     |
| $h_{R_i}$            | $\begin{cases} 1 & \text{if } a_j \in R_i \\ 0 & \text{if } a_j \notin R_i \end{cases}$ | $\begin{cases} 1 & \text{if } a_j \in R_i \\ 0 & \text{if } a_j \notin R_i \end{cases}$          | $-3r(s^i_t, s^j_t)\tau\gamma^3 3^{3/2}/R^3$                                                      |
| $h_i$                | $\{c^i_t\} \cdot h_{R_i}$                                                        | $\{v^e_x, v^e_y\} \cdot h_{R_i}$                                                                  | $\{x^i_t, y^i_t\} \cdot h_{R_i}$                                                                  |
| $g$                  | $\{c^i_t\}$                                                                        | $\{v^e_x, v^e_y\}$                                                                                  | $\{x^i_t, y^i_t\}$                                                                                  |

System formulation from problem definition section of main manuscript is applied to simulated model systems. Here, $h = \sum_j h_j$, $h_x = \{x\}$ directional component of $h$, $h_y = \{y\}$ directional component of $h$, and $|R_i|$ denotes the number of element of set $R_i$. $r(s^i_t, s^j_t)$ represents distance between two agent’s position, while $\theta(s^i_t, s^j_t)$ represent respective angle of $j$th agent to $i$th agent. In case of AOUP, $t + 1$ becomes $t + dt$ since original model is governed by continuous differential equation. Descriptions of variables that constitute each system are reported in SI appendix.

Table 4: Implementation details of models for sample systems

| System                          | Input data dims. | # of Attention head | Attention head dims. | Neural attention blocks       |
|---------------------------------|------------------|---------------------|----------------------|-----------------------------|
| 1. Cellular Automata            | 3                | 1                   | 20                   | $[32, 16, 1]$               |
| 2. Vicsek Model                 | 4                | 3                   | 20                   | $[32, 32, 1]$               |
| 3. Active Ornstein-Uhlenbeck Particle | 4 + 1*       | 3                   | 20                   | $[32 + 1*, 32, 1]$          |
| 4. Chimney Swift                | 6 + 1**          | 1                   | 30                   | $[16, 8, 1]$                |

*: global variable ($R$), **: indicator variable
Table 5: Comparison between different attention mechanisms in Vicsek Model

| Attention           | Train loss (NLL) | Test Loss (NLL) |
|---------------------|------------------|-----------------|
| Additive attention  | -0.694           | -0.672          |
| Multiplicative      | -0.778           | -0.743          |
| Neural attention    | **-1.013**       | **-1.021**      |

Figure 6: (A) Functions of *smoothed* version of interaction range, sigmoid models with various smoothing parameter $b$. (B) Performance comparison of VAINS, GAT and AgentNet compared to NLL loss from groundtruth.

$14 \times 14$ grid with uniformly random initial cell state and updated inner square grid of $12 \times 12$ to avoid a periodic boundary problem. We simulated 1,000 sets of samples for demonstration, 800 samples for training and 200 samples for test. We report that fewer samples such as 500 or 300 samples also resulted in a perfectly trained model with 100% test accuracy. As depicted in Fig. 3b in the main manuscript, we further tested the validity of trained model with augmented test data. Each target cell along with 8 neighbor cells yield total $2^9 = 512$ possible microstates. We located $3 \times 3$ microstate template at random position on the grid cell, initialized to random cell states and produced AgentNet output. If the model correctly learned the transition rule, it would result in theoretical output assigned by the transition rule of CA regardless of its position and other irrelevant cell states. Fig. 2 in the main manuscript shows the AgentNet output for each microstate with 1,000 different environments, which verifies the performance of AgentNet.

**Vicsek model**

Vicsek model (CM) [9] assumes that flocking occurs due to velocity alignment with neighbors. Among the many variants, we implemented the simplest model with alignment term and positional gaussian noise. (Note that this is different from originally proposed model [9], which used angular gaussian noise instead.) In VM, $i$th agent interacts with $j$th agent if the distance between two agents, $r(s_i^t, s_j^t)$ is smaller than certain range $r_c$ and the absolute value of angle between heading direction of $i$th agent and position of $j$th agent, $\theta(s_i^t, s_j^t)$ is smaller than certain angle $\theta_c$. This interaction range models the limit in sight range of living organisms, result in the form of a circular sector. In VM, $i$th agent averages velocity among its interacting neighbors $R_i$ and add gaussian noise $N(0, \sigma)$ to compute its velocity, described as follows.

$$v_i^t = (v_i^{t+1} + \sum_{a_j \in R_i} v_j) / (|R_i| + 1) + N(0, \sigma).$$
This formula is equivalent to \((\sum_{i} r_i^2 v_i)/|R_t^*| + \mathcal{N}(0, \sigma)\) where \(R_t^* = R_t \cup a_t\).

AgentNet for VM aims to predict the position of the next time step, which is a sum of the current position and calculated velocity. We simulated 2,000 sets of samples for demonstration, 1600 samples for training and 400 samples for test. In our simulation, \(r_c = 1, \theta_c = 120^\circ\), and standard deviation of noise \(\sigma = 0.2\).

Active Ornstein-Uhlenbeck Particle

For AOUP dataset, 100 particles were uniformly spread on the circle of radius 5, and initial speeds were sampled from uniform distribution \(U(0, 0.05)\). We implemented Euler-mayurama \([66]\) method with timestep \(dt = 0.01\) to numerically simulate the trajectory of AOUP. The data and label points were further subsampled from simulated trajectory with frequency 10Hz, which means every 1 out of 10 subsequent datapoints were chosen. In sense of time, our model receives 0.8 seconds of observing data and subject to predict following 1.2 seconds of trajectory. Following constacts were adopted for simulation: \(\gamma = 1, \tau = 0.5, k = 0.1, D_a = 0.04, T = 0.1\). We have found that our model is robust for change of system constants, showed similar performance with different constant values.

We employed teacher forcing \([67]\) to train LSTM-based AgentNet, which is a technique that feeds ground-truth label into consequent LSTM cell instead of sampled output in the early stage of training. This is useful to stabilize the training of trajectory prediction since the prediction depends on the last output which typically explodes to meaningless values in the early, untrained stage. We set an initial 50 epoch as a teaching period that the possibility of using the ground-truth label is \(1 - \text{epoch}/50\). This gradually decreasing possibility becomes 0 at epoch 50, and do not use ground-truth afterward.

For evaluation, linear extrapolation along with naive LSTM is selected as baselines. In the case of extrapolation, \(x\) and \(y\) coordinates of previous 8 steps are extrapolated through time and consecutive 12 steps are recorded. Naive LSTM used same state variables \((x, y, v_x, v_y)\) and same output structure, but only have LSTM encoder and MLP decoder, missing an attention core. This implies that there are no effect of interactions with others for naive LSTM. Averaged Displacement Error (ADE) is calculated by taking average of euclidean distances from groundtruth to predicted coordinates for all 12 steps. Final Displacement Error (FDE) only takes the averages of final (12th step) error.

Chimney Swift flock trajectory

Original paper \([11]\) aimed to focus on collective behavior at the landing sequence of chimney swift flock. The whole dataset can be divided into three parts: (1) initial stage where birds are starting to gather, (2) birds flock are formed and show collective spinning, and (3) landing on the chimney. In this study, we used the second portion (file B) of the data since we are interested in general bird flocking rather than a specific landing sequence. Among 30 minutes (=54000f) of trajectory data, we employed around 10 minutes (=18000f) of frames and constructed dataset with 15f * 10 = 150f each, 75f apart from each other. Exact details about dataset and statistics can be found at \([11]\).

In the case of CS, there is a problem of unbalanced labels since not every sample has full 10-step (5s) trajectories, as mentioned in the main manuscript. Thus, we checked the number of agents present at certain steps and calculated a weighted loss to strengthen the effect of cases with fewer birds (typically, the case of higher time step has a smaller number of constituent since many trajectories end early.).

Since every trajectory starts and ends at a different time steps, we take an average of bird displacement error where its own starting point is regarded as time step 0. For instance, if the trajectory of bird 1 spans from time step 0 to 3 and the ones of bird 2 spans from 4 to 6, error calculated at bird 1, step 2 and bird 2, step 6 will be samely treated as displacement error at time step 2 since both steps are 2nd steps with respect to their own starting point. Also, since there were trajectories only lasted 2 time steps (= 1.0s), we cannot apply linear regression for those trajectories. Instead, we linearly extrapolated the trajectories by employing given velocity at first time step.

2. Implementation details of AgentNet

Neural model

The encoder and decoder layers of AgentNet is composed of Multi-Layer Perceptrons (MLP). The dimension notation such as \([32, 16, 1]\) means that the model is consists of three perceptron layers with 32, 16 and 1 neurons in each layer. Also, dims. is an abbreviation of dimensions.

All of the encoding layers of AgentNet is composed of \([\text{Input dims}, 256, 256, \text{Attention dims.} \times \# \text{of Attentions}]\). Here, input dimensions are chosen as sum of the number of state variables and additional variables such as global variable (as in AgentNet for AOUP) and indicator variable (as in AOUP for CS). The form of the final dimension indicates that each output of encoder (key, query, and value) will be processed separately.
With these outputs and (additional) global variables, neural attention is applied and attention coefficients $e_{ij}$ are calculated. (Details of neural attention is explained in section 3 of SI. appendix.) We apply additional LeakyReLU nonlinearity (with a negative slope of 0.2) to the attention coefficients and normalize them with softmax, following [5].

After attentions are multiplied to respective values and averaged, we concatenate the (original target agent’s) value and its averaged attention-weighted values (from others) and feeds it into the decoder. Since two tensors are concatenated, the last dimension of this tensor has twice the length of the original dimension of value tensor. Decoder consists of $[2 \times \text{ value dims.,} 128, 128, \text{ output dims.}]$. Note that the dimension of the value vector is the same as $[\text{Attention dims.} \times \# \text{ of Attentions}]$, since it is an output of the encoder.

In the stochastic setting, decoded tensor further feeds into other layers to obtain sufficient statistics for the probabilistic distribution. In this paper, those statistics are means and covariance matrices. Layers for theses values are consist of $[\text{output dims.,} 64, 64, \text{ corresponding number of variables}]$. For instance, a 6-dimensional covariance matrix is uniquely decided with 21 variables, thus the final dimension of covariance layer is 21.

In the case of the target system with probable time correlations, we adopted Long Short-Term Memory (LSTM) as an encoder to capture those correlations. Hidden states and cell states have 128 dims. each and initialized by additional MLPs that jointly trained with the main module. As explained in the main manuscript, AgentNet checks each time step whether an agent is new and present. If an agent is newly entered, new LSTM hidden states are initialized. Otherwise, hidden states succeeded from the previous result.

### Training

All of the training used 2 to 10 NVIDIA TITAN V GPUs, the longest training for single model took less than 2 days. ReLU activations and Adam Optimizer [64] are used for construction of model and training. The learning rate was set to 0.0005 and decreased to 70% of previous value when the test loss remains still for 50 epochs. Table 1 shows further details of the model for each system, including the number of attention heads.

### 3. Advantages of Neural attention

Neural attention needs greater number of parameters to optimize, but showed greater performance on predicting complex agent compared to existing attention mechanisms. Table 2 shows the performance of AgentNet for Vicsek Model (VM), each employed different attention mechanisms to calculate attention between $i$th and $j$th agents, $\alpha_{ij}$. Here, we used transformer [65] architecture for all three mechanisms which separates key $k$, query $q$ and value $v$. Additive mechanism employs three $d \times d$ weight matrices $w_1, w_2, w_3$ to compute attention weight as $w_3(\sigma(w_1 k_i, w_2 q_j))$, where $d$ is a dimension for output vector, $\sigma$ is a nonlinear activation function, $k_i$ is a key for $i$th agent and $q_j$ is a query for $j$th agent. Multiplicative mechanism calculates attention weight with inner product as $k_i \cdot q_j$ with some normalization constant, and broadly used to handle sequential data such as a natural language.

In contrast, neural attention uses multiple MLP layers $A_\theta$, parametrized by $\theta$, to compute attention.

$$\alpha_{ij} = A_\theta(k_i \| q_j \| u) \quad (9)$$

Here, $\|$ indicates the concatenation of two vectors and $u$ is the vector of global variables. Note that the additive mechanism is technically the same as a single layer of perceptrons. Table 3 shows the results of AgentNet for VM that employs different attention mechanisms. (In this case and following demonstration, the system has 100 agents compared to 300 agents of the main manuscript version. This results in slightly lower NLL value, $-1.013$, compared to the one reported in the manuscript, $-0.856$ since the system with lower density is easier to predict.) We observed that both additive and multiplicative attention cannot fully capture the nonlinear and complex interaction range of complex systems as neural attention does.

One possible reason for the outperformance of neural attention is that the interaction range of a complex system is far more nonlinear and complicated that conventional attention mechanisms are relatively under-parametrized for such interaction range. This surmise is further supported if the performance gap decreases as the interaction boundary becomes more linear. We experimented with smoothed version Vicsek model, where interaction strength is defined as a sigmoid function $s(x) = 1/(1 + \exp(b(x - a)))$. Fig. S1 shows the performances of VAIN(exponential based attention from [6]), GAT (conventional transformer) and AgentNet (neural attention) with different $b$ when $a = 1$. Note that original interaction boundary coincides with $b \rightarrow \infty$ case. The results show the difference between two mechanisms scales with $b$, which underpins the aforementioned nonlinearity hypothesis.
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