Learning Collective Behaviors from Observation

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Abstract

Collective behaviors (aka self organization), such as clustering, flocking, milling, swarming, and synchronization, occur naturally in instantaneous magnetization, super conductivity, crystal formation, cell aggregation, social behaviors of insets (bees, ants, locusts) and animals, market behaviors, traffic patterns, and more (see [1] and the 2022 AMS Josiah Willard Gibbs Lecture on Collective Dynamics¹). It is a challenging task to understand such behaviors from the mathematical point of view. We offer a series of statistical/machine learning methods to explain collective behaviors from observation data.

Consider a simple first-order system of N agents², where each agent is assigned a time-dependent state vector $\mathbf{x}_i(t) \in \mathbb{R}^d$ (\mathbf{x}_i can represent position, velocity, phase, emotion, health status, etc.), the temporal change of $\mathbf{x}_i(t)$ is trying to minimize a special system energy which has symmetries and other desired properties (shown by observation and other experimental data), which is given as follows

$$\dot{\mathbf{x}}_i(t) = \frac{1}{N} \sum_{j=1, j \neq i}^N \phi(\left|\mathbf{x}_j(t) - \mathbf{x}_i(t)\right|) (\mathbf{x}_j(t) - \mathbf{x}_i(t)), \quad i = 1, \cdots, N.$$

Here $\phi : \mathbb{R}^+ \to \mathbb{R}$ is known as the **interaction law** governing how agent j would influence the change of $\mathbf{x}_i(t)$. Current research on collective dynamics focuses on deducing the desired behavior (clustering, flocking, etc.) from a known class of interaction functions. However, when the trajectory data, i.e. $\{\mathbf{x}_i(t), \dot{\mathbf{x}}_i(t)\}_{i=1}^N$ for $t \in [0, T]$, is given with all the necessary information except ϕ , can we learn the interaction law, ϕ , from this set of data?

Concatenating the \mathbf{x}_i into one big vector, i.e. letting

$$\mathbf{X}_{t} = \begin{bmatrix} \vdots \\ \mathbf{x}_{i}(t) \\ \vdots \end{bmatrix} \in \mathbb{R}^{D} \quad \text{and} \quad \mathbf{f}_{\phi}(\mathbf{x}_{t}) = \begin{bmatrix} \frac{1}{N} \sum_{j=1, j \neq i}^{N} \phi(|\mathbf{x}_{j}(t) - \mathbf{x}_{i}(t)|)(\mathbf{x}_{j}(t) - \mathbf{x}_{i}(t)) \\ \vdots \end{bmatrix}, \quad D = Nd \gg 1,$$

then our learning problem could be re-written as a regression problem, i.e. finding \mathbf{f}_{ϕ} such that $\dot{\mathbf{X}}_t = \mathbf{f}_{\phi}(\mathbf{X}_t)$, given $\{\mathbf{X}_t, \dot{\mathbf{X}}_t\}$ for $t \in [0, T]$. However the lack of data independence and the high dimensionality of observation data prevent us from taking the normal regression route (or other approaches for learning dynamical systems, such as SINDy, Neural ODEs, PINN, etc). Therefore, we design an error functional (which is similar to a loss function in training deep neural networks) which exploits the special structure of the collective dynamics. In [2], a convergence theory of our data-driven approach is established and the convergence is shown to be optimal and independent of the dimension of the observation data. We also consider second-order systems together with interaction for the agent with its surrounding environments, similar to those used in model flocking, milling and swarming, we develop a learning theory in [6] and investigated the steady state behaviors of our estimated dynamics (from first- and second-order observation data) in [3]. When the state of the i^{th} lives on a

¹Link: https://youtu.be/AenZz60oj2g

²Agents here can be referred to as particles, cells, robots, animals, etc.

Riemannian manifold (those locally behaving like an Euclidean space, i.e. a 2D-sphere), we present a convergent theory preserving the geometric property of the data in [4]. The assumption that the interaction kernel ϕ has to be radially, i.e. depending on the pairwise distance variable $r_{i,i} = |\mathbf{x}_i - \mathbf{x}_i|$, is too restrictive and not realistic for biological systems. We relax such restriction and assume that the interaction variables also become unknown, i.e. we have to learn $\Phi(\mathbf{x}_i, \mathbf{x}_i)$ instead of $\phi(r_{i,i})$ with $r_{i,j} = |\mathbf{x}_j - \mathbf{x}_i|$. Φ is a 2d-dimensional function $(d \gg 1)$ making the direct application of our original learning approach computationally prohibitive. We combine a Multiplicatively Perturbed Least Square to learn dimension-reduced representation of Φ with our original approach, then we are able to learn Φ effectively. Details can be found in [5]. With our learning theories being theoretically proven and supported on various applications using simulated observation data, we decide to test the theories on real observation data, in particular, 500 years of daily position/velocity data of the Sun, 8 major planets, and the Moon of the Earth from NASA JPL's Horizons database (DS430/431). We overcome the difficulties of missing acceleration data, long-time integration of a Hamiltonian system, large data set; and we are able to produce a data-driven collective dynamics model with fewer assumptions than Newton's Universal Law of Gravitation and the capability of re-producing the perihelion pression rates (a sensitive measure of the accuracy of the prediction of the planets' trajectories) for Mars, Mercury and the Moon close to the JPL's data. Our model can also be used to estimate the masses of the celestial bodies (including Sun, the planets, etc.) upto 2-digit relative accuracy. Details can be found in [7]. Learning theories on second-order general relativistic models and from observation data at steady states are on going.

We are also actively developing newer collective dynamics models such as the emergence of line formation in [8], concurrent emergence of several collective behaviors in [9]. A new model on random movements of cell/bacteria is also being investigated.

References:

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