An information theoretical approach to the inverse problem in collective animal behaviour

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The inverse problem in collective animal behaviour consists in finding the forces that govern the motion, given the observed trajectories. Here, correlations between dynamical variables and the associated forces are measured using Information Theory, by means of an entropy definition. The entropy values are used in two ways. Firstly, for recognizing important variables used later in a regression method; and secondly, as a function independent parameter estimation method. The approach is successfully tested by reconstructing the equations of motion given data generated with simulations.

I. INTRODUCTION

Groups of animals often exhibit fascinating features. Motion could be either coordinated or display abrupt changes in direction. Under pressure, like the presence of a predator, the same group may swirl as a fluid [1].

In Physics and Chemistry, fundamental laws can guide the modeling process. The motion of living organisms, however, lacks such fundamental laws. That is why it is of great importance inferring the underlying dynamics from observations. This is known as the inverse problem.

Models of self-propelled particles that self-organize under pairwise interactions have been proposed [2] [3]. However, fitting those models to real data has not yet been successful. Force Matching methods have been used [4] for aligning forces with additively separable terms, proportional to $f(r_{12})\boldsymbol{r}_{12}$, and $\boldsymbol{v}_{12}$, where $\boldsymbol{r}_{12}$ is the vector between two individuals and $\boldsymbol{v}_{12}$ is the difference of its velocities. Here, more general functions of combinations of those variables are explored.

Any modeling approach that involves regression assumes that we know, beforehand, the arguments of the functions to fit. Let us assume first, for the sake of simplicity, that the system is purely mechanical. For N individuals interacting in a d-dimensional configuration space, the upper limit for the number of independent variables is $2dN$. A polynomial fit of degree m would require coefficients for the m terms of each variable, plus coefficients for all the mixed, or interaction terms. Therefore, this brute-force approach is useless in practice, unless we have extremely large sets of data.

Information theory provides powerful tools for analysing correlations between data, and the study of correlations between effects and their possible causes sounds like a good starting point for the inverse problem. Entropy, in this formalism, can be thought of as the external information required to represent a system, if we use a suitable definition. Hence, with the entropy of the rule that assigns the magnitude to infer to the dependent variables that we are considering, we can measure how random the system looks under those particular variables, or description. The lower the randomness, the better the description of that system. In this context, correlations mean predictability. Information theory will be used to measure how relevant are certain sets of variables to the dynamics. These measures will have the property of being independent of the function to fit.

Traditional curve fitting methods are based on polynomial fitting. In many interesting cases, the arguments of the function to fit are itself functions of the dynamical variables and parameters. If we simply perform polynomial fitting, the parameters will be mixed with the coefficients of the fitting, making difficult any information extraction. A function independent method has two main advantages. It allows us to test educated guesses about the form of the arguments. And finally, it helps us discovering parameters in a cleaner way.

As I discuss below, under an incomplete set of variables, the system will display higher entropy than under the complete set. The entropy remaining when the system is observed under the complete set of variables –or an equivalent one– is a measure of the noise in the system. In the context of collective animal behaviour, noise has been proposed as the control parameter that drives the system into a critical state [5], in which correlation length increases dramatically. Hence, it is useful to have a noise measure that is function independent.

The whole procedure used here starts by obtaining the trajectories. Then, by numerical differentiation all the required dyanmical variables can be calculated. After that, I use the entropy for finding the relevant variables and the parameters. Finally, the system is separated in different regimes, in order to recover the equations of motion by regression.

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II. THEORY

Let $D = \{D_1, D_2, ..., D_r\}$ be a set of r independent variables of a discrete (or discretised) dynamical system, consisting of N individuals in a configuration space of dimension d. The system can be either stochastic or deterministic. At every time step t, the state of the individual X_i is $\boldsymbol{X}_i^t = (X_{i1}^t, \ldots, X_{ir}^t)$. Define the neighbourhood (dependent on d) of individual i at time t of extension b, as the set of b closest individuals to $\boldsymbol{X_i}$ to be $\sigma_{i,b}^t = \sigma(\boldsymbol{X}_i^t; b)$.

Consider a space of outcomes $O = \{O_1, O_2, ..., O_m\}$ to be predicted, and the probabilistic description

$$P\big(O_j|\sigma_{i,b}^t\big)$$

O for instance could be the next state of a Cellular Automata if σ represents the previous neighbouring states, or the force exerted on a particle if σ are the surrounding particles. P can be constructed by observing the system, or it can be known a priori if we are working with a model. If this is the case, we will say that we know the *true* probabilities of the system, and that we have the *correct* description of the system.

At time t, we define the entropy production of the prediction using the description D as

$$S^t(X, O) = \lim_{b\to\infty} \sum_i P\big(\sigma_{i,b}^t\big) \sum_j P\big(O_j|\sigma_{i,b}^t\big) \log \frac{1}{P\big(O_j|\sigma_{i,b}^t\big)}$$

By definition, S measures how stochastic is the system under the description D, and hence, the stochastic component plus our possible lack of information about the description. It measures on average how multivalued is the outcome of a dynamical state.

By construction, S can be considered a tool for characterising the best description D, as the smallest set of independent variables that minimises S. However, for it to be considered a definition, it must be proven that if a correct set D exists, then (i) and (ii) hold:

(i) For every t and b, if $D_1 \subseteq D \Longrightarrow S^t(D1) \geq S^t(D)$

(ii) For every t and b, if $D \subseteq D_2 \Longrightarrow S^t(D) = S^t(D_2)$ if the added degrees of freedom are non-trivial and with statistically enough information.

Those statements can be proven easily, if we know the dynamics, i.e. D and the true probabilities $P\big(O_j|\sigma_{i,b}^t\big)$. It is intuitive if we consider that ignoring variables produces less narrow probability distributions for the outcome given an income, and therefore entropy increases. Adding variables produces more states, but if the number of points is large, the probability distributions will not change, because the added variables are independent and hence not taken into account for assigning the outcome.

III. MODEL

The approach discussed in the previous section was tested with a very simple model of fish in $2D$ that exhibits swirling and boundary behaviour similar to real systems. The aim is to construct a full model and then recover the equations of motion from the trajectories only.

In this model, for each pair of animals, the following value is computed

$$\eta = \sqrt{(r_x + T\Delta v_x)^2 + (r_y + T\Delta v_y)^2}$$

Where $\boldsymbol{r}$ is the vector between the animals, $\boldsymbol{\Delta v}$ is the difference in their velocity and T is a reference time. Therefore, η measures how will the distance between both animals be after a time T if they keep their velocities constant. If L is a reference distance, a force proportional to an odd power p of $\eta - L$ is then exerted on the fish. The direction of the force is in that of the maximum growth of $\sigma = \eta - L$, if σ is positive, and in the perpendicular direction if σ is negative. This is a very simple instance of how a living organism can modulate its velocity in a group, keeping a certain distance from the others while copying their speed, and running away if they are too close. It sounds plausible that an animal acts in advance, choosing a behaviour depending on the distance that will separate both after some time, rather than the current distance. Beyond certain distance called the interaction range, the animals do not interact.

For each animal, there is also a self-propelling force and a dragging force as in [3]. The self-propelling force is proportional to the velocity $\boldsymbol{v}$ of the animal, and the dragging force is proportional to $v^2\boldsymbol{v}$.

The boundary is considered a potential well. The effect due to the boundary is proportional to the product of the well and the projection of the velocity on the outward normal of the surface. As the points near the boundary will be disregarded, the form of the force due to the boundary is not important. However, the presence of a boundary is important for a reason. After removing the points near the boundary, a simulation as well as a real run are both equivalent to several runs with different initial conditions.

In this model, interactions are pairwise and noise is present in the form of a force $\boldsymbol{\chi}$. Where $\boldsymbol{\chi}$ is normally distributed, with mean zero and variance constant in time.

The total force is then, for points away from the boundary, with $\sigma > 0$ and within the interaction range:

$$\boldsymbol{F} = (a - bv^2)\boldsymbol{v} + \frac{(\eta - L)^p}{\eta}\hat{\boldsymbol{\eta}} + \boldsymbol{\chi}$$

Conversely, if $\sigma < 0$

$$\boldsymbol{F} = (a - bv^2)\boldsymbol{v} + \frac{(\eta - L)^p}{\eta}\hat{\boldsymbol{\eta}}^{\perp} + \boldsymbol{\chi}$$

This model, although biologically simple, presents challenging features for the inverse problem.

IV. IMPLEMENTATION

Let us suppose we do not know the dynamics. The original equations of motion can be recovered from observations provided we make some assumptions and we have a set of measurements. The data required is the trajectory of each fish parametrized by time. After numerical differentiation, all required dynamical variables can be computed from this set. Not all the assumptions I will make are restrictive, some of them are on the contrary, including possible features that usually mechanical systems do not exhibit.

The assumptions I will make are:

1. Interactions are pairwise so the forces are additive. Hence, all the dynamical information is contained in the trajectories of two animals.
2. The noise component is drawn from a distribution constant in time.
3. There can be a repulsive and an attractive zone, that are possible to estimate from measurements, as in [6]. Here, a less general way of knowing this regions will be used.
4. The part of the force due to the interaction of the animals is a general function of a linear combination $\boldsymbol{\rho} = c_1\boldsymbol{r}_{12} + c_2\Delta\boldsymbol{v}$ of the distance between them and the difference of their velocities. A reasonable assumption given the observed tendency of the animals to stay together and align their velocity.
5. The form of the force in the repulsive region may change in both, direction and magnitude, respect to the form of the force in the attractive region.
6. The effect of the boundary away from it is negligible.
7. There is a self-propelling force and a dragging force along the direction of the own velocity, and dependent on the own speed only.
8. Beyond a distance called the interaction range, animals do not interact. This range can be estimated from observations. This is not necessary for the method to succeed. However, if the interaction drops dramatically after some distance, taking this into account leads to a faster convergence.

There is another useful assumption, although not entirely necessary. In an isotropic medium, the relevant part of $\boldsymbol{\rho}$ is its norm ρ. We can test the assumption by measuring the entropy of the system under the angular part of $\boldsymbol{\rho}$, or by evaluating the final fit. In brief, for an isotropic medium, considering all the previous assumptions, the following force is being proposed for the attractive regime

$$\boldsymbol{F} = f(v)\boldsymbol{v} + g(\rho)R(\boldsymbol{\rho}) + \boldsymbol{\chi} = \boldsymbol{F}_{\boldsymbol{v}} + \boldsymbol{F}_{\boldsymbol{\rho}} + \boldsymbol{\chi} \qquad (1)$$

And for the repulsive regime

$$\boldsymbol{F} = f(v)\boldsymbol{v} + g_2(\rho)R_2(\boldsymbol{\rho}) + \boldsymbol{\chi}$$

Where R and R_2 are rotation operators that depend on whether we are in the attractive or in the repulsive regime. Although it is more general to include these operators, they might be constant and $g = g_2$ if g itself has an attractive-repulsive nature. Although the variable $\boldsymbol{\rho}$ is a linear combination of $\boldsymbol{r}_{12}$ and $\Delta\boldsymbol{v}$, it is a step further in generalization to consider arbitrary functions of its norm.

Observing real systems with different behaviour can lead to different assumptions. As the possibility of testing all the assumptions exists, the procedure can be easily extended if observations suggest otherwise. Observations will actually shape the assumptions. Some of these changes could lead to excessive computational or information requirements, while others will not.

If we suspect that any other variable is important for the dynamics, we can check whether the entropy of the outcome is reduced or not with this variable, compared to the entropy obtained by using the other variables. Depending on the situation, it is useful to consider the entropy under groups of variables, or the entropy under single variables.

A system comprised of two fish is far from being statistically significant. Nevertheless, if noise distribution is constant in time, we can perform time averages instead of spatial averages. The entropy equation is then reduced to

$$S(I,O) = \sum_t P(I_t) \sum_j P(O_j|I_t) \log \frac{1}{P(O_j|I_t)}$$

Where I_t is an n-dimensional point whose coordinates are the n dynamical variables to consider, at time t. O_j is the projection of the total force due to one of the animals along a particular direction, at time t.

S can be used to know if our set of variables is complete, by comparing the entropy of the system with the entropy under the full set, but that would be computationally expensive. A more important feature is that it can be used as a function independent parameter estimator. By function independent it should be understood that, for instance, if F is the magnitude of the force corresponding to one of the individuals, for ρ as defined above

$$S[\xi(\rho), F] = S[\rho, F]$$

For any function ξ, in particular $\xi = g$. Hence, we can find c_1 and c_2 by minimizing $S[\rho, F]$ in the parameter space of ρ.

With only two parameters in this particular case, and because of this function independence:

$$S[\|c_1 \boldsymbol{r}_{12} + c_2 \Delta \boldsymbol{v}\|, F] = S[\|\boldsymbol{r}_{12} + \frac{c_2}{c_1} \Delta \boldsymbol{v}\|, F] \qquad (2)$$

And therefore, we only need to find one parameter. A later regression will multiply this term by a proper constant so that c_1 and c_2 are both known.

V. RESULTS AND DISCUSSION

In order to find c_1 and c_2, I searched for the value of $\frac{c_2}{c_1}$ that minimized equation (2).

In figure 1, $S[\rho(\boldsymbol{r}_{12}, \Delta \boldsymbol{v}; \frac{c_2}{c_1}), F]$ is plotted as a function of $\frac{c_2}{c_1}$ for a system in which the true value is $\frac{c_2}{c_1} = 0.1$

For finding f, the same procedure can be performed on powers of the speed. f can be found as well by regression if we already know $\boldsymbol{\rho}$ and there is no rotation operator, or if we know the operator beforehand. In order to find it by regression, we also need to be sure that the force only depends on $\boldsymbol{v}$ and $\boldsymbol{\rho}$. Conversely, the Information Theory approach does not require the knowledge of $\boldsymbol{\rho}$ or the rotation operator if it exists, but it needs to be carried out on a projection of the force in any direction, given that for the total force associated to the velocity

$$S[F_v, F] = S[f(v)v, F] = S[\boldsymbol{v}, F]$$

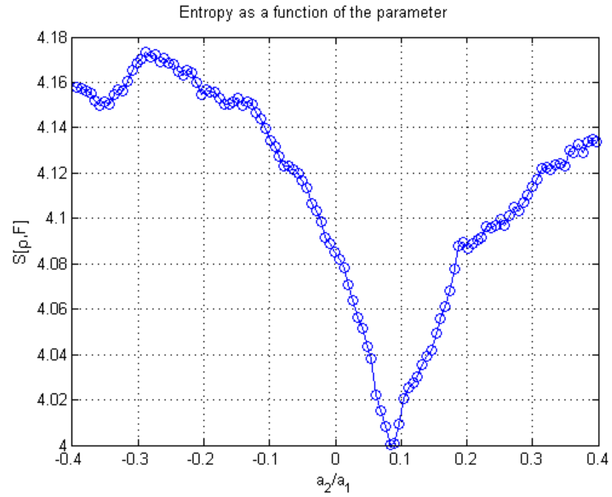

FIG. 1. In this plot, $\frac{a_2}{a_1}$, the parameter of ρ, was varied until the value that minimized S was found. The true value of was 0.1

Therefore, all the sets of parameters yield similar entropy estimates.

After knowing f and $\boldsymbol{\rho}$, up to a multiplicative constant, we proceed to find the rotation operator, if any. First we need to remove the points near the boundary, for a cleaner procedure. By knowing f, as we can compute from the trajectories $\boldsymbol{v}$ and $\boldsymbol{F}$, we can calculate $\boldsymbol{F_\rho}$ from (1).

Figure 2 shows a plot of the cosine of the angle between $\boldsymbol{\rho}$ and $\boldsymbol{F}_\rho$. The plot is noisy but we can observe that for $\rho > 2$ the force is parallel (attractive regime) and for $\rho < 2$ the force is perpendicular (repulsive regime). The absence of a rotation operator would produce a continuous value. If the direction of the force were not a function of ρ, it would be also observed in this plot.

Likewise, a plot of r_{12} vs F_ρ allows us to decide whether there is an interaction range or not.

Finally we are in conditions of making a regression for finding g. We need a second filtering. Now we need to keep either the points in the attractive regime, or the points in the repulsive regime. Figure 3 shows an added variable plot of the multivariate regression:

$$F_x \propto f v_x + \sum_i \rho^i \rho_x$$

In the attractive regime. The dispersion is due to the noise. Points are scattered symmetrically, suggesting a successful regression. A non-considered force would appear in this plot as a different trend. If the angular component of $\boldsymbol{\rho}$ were important, here it will be evident.

With the coefficients of this fit, it is straightforward to

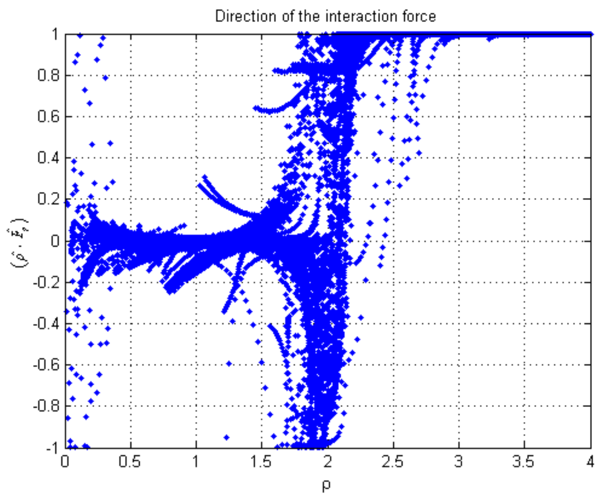

FIG. 2. The cosine of the angle between $\boldsymbol{\rho}$ and $\boldsymbol{F}_\rho$.

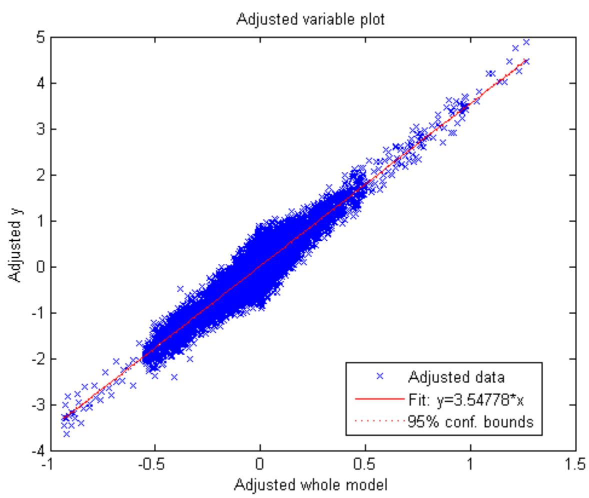

FIG. 3. Adjusted variable plot for the multivariate regresion of the force in the direction of $\hat{x}$.

reconstruct the equations of motion, as we can know the true values of $\boldsymbol{F}_v$ and $\boldsymbol{F}_\rho$. The repulsive regime can be treated alike.

VI. SCOPES, LIMITATIONS AND NUMERICAL CONSIDERATIONS

It is a rather remarkable feature that the parameter estimation did not require filtering data or separating the system into different regimes. For instance, even knowing that $\boldsymbol{F}_v = (a - bv^2)\boldsymbol{v}$, an attempt to find a and b by regression without knowing $\boldsymbol{F}_\rho$ would be unsuccessful, while it was possible with the Information Theory approach. This fundamental difference, perhaps, is due to the fact that regression works when the unknown or ignored part is certain kind of noise. The Information Theory approach, on the other hand, still works if the unknown or ignored part is not strongly correlated to the part we are analysing.

One must be careful while proceeding this way. If we want to estimate $S[\rho, F]$, formally, we need to consider $S[(\rho, \boldsymbol{I}), F]$ where $\boldsymbol{I}$ is the remaining dynamical information. However, we have assumed that $\boldsymbol{F} = \boldsymbol{F}(\boldsymbol{\rho}, \boldsymbol{v})$, and as $\boldsymbol{\rho}$ is a function of the velocity differences, $\boldsymbol{v}$ is not strongly correlated to $\boldsymbol{\rho}$. When one variable appears explicitly in other, we need to be careful while choosing the arguments of S. Clearly, the number of states grows exponentially with the number of dimensions considered, therefore, when possible, it is convenient to find a description with non-overlapping variables, or at least with not strongly correlated variables. In figure 1 the true value of the parameter is 0.1, we can observe a small deviation towards the left because we are not using information about the other variables. A small trade-off for avoiding the explosion in the number of states when we include more dimensions.

As in any numerical method, the size of the bins is important. A much faster convergence is achieved by considering bins with equal number of points, rather than bins of equal size. This is straightforward to implement when the argument of S is one-dimensional. For higher dimension, something useful and easy to implement is to divide each dimension in pieces of equal number of points and perform the average only with those n-dimensional bins whose number of points is greater than a threshold.

As a reference, figure 1 has 115 points, each of them is an evaluation of S. The system is the trajectory of two individuals, having 100000 points each one. The number of bins used to estimate S was 200. The total run time in a regular computer was 109 seconds.

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