Modeling Heterogeneity in Networks using Polynomial Chaos

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Abstract

Using the dynamics of information propagation on a network as our illustrative example, we present and discuss a systematic approach to quantifying *heterogeneity* and its propagation that borrows established tools from Uncertainty Quantification, specifically, the use of Polynomial Chaos. The crucial assumption underlying this mathematical and computational "technology transfer" is that the evolving states of the nodes in a network quickly become correlated with the corresponding node "identities": features of the nodes imparted by the network structure (e.g. the node degree, the node clustering coefficient). The node dynamics thus depend on *heterogeneous* (rather than *uncertain*) parameters, whose distribution over the network results from the network structure. Knowing these distributions allows us to obtain an efficient coarse-grained representation of the network state in terms of the expansion coefficients in suitable orthogonal polynomials. This representation is closely related to mathematical/computational tools for uncertainty quantification (the Polynomial Chaos approach and its associated numerical techniques). The Polynomial Chaos coefficients provide a set of good collective variables for the observation of dynamics on a network, and subsequently, for the implementation of reduced dynamic models of it. We demonstrate this idea by performing coarse-grained computations of the nonlinear dynamics of information propagation on our illustrative network model using the Equation-Free approach.

Keywords: coarse-graining, social networks, Equation-Free approach, UQ, Polynomial Chaos

1. Introduction

Our purpose in this paper is to establish a link between Uncertainty Quantification in dynamical systems depending on (uncertain) parameters, and Het-

erogeneity Quantification in dynamical systems consisting of (many) individual dynamical units coupled in a network. These units differ in the way they are structurally linked to form the network; their "structural identities" are heterogeneous, and the distribution of these heterogeneities derives from the network structure itself.

Network models are increasingly being used to study large, complex real life systems in a variety of contexts such as the internet, chemical and biochemical reaction networks, social networks and more [2, 3, 4, 5, 6]. A network is a mathematical representation of individual subsystems called nodes (or vertices), which are connected to one another through edges (or links). In the specific example of a social network the nodes represent people, while the edges connecting them represent relationships (friendships, coauthorships, etc.) between them. The following references provide useful reviews of basic network concepts and of the study of dynamics of evolving networks [7, 8, 9, 10, 11, 12]. Dynamic evolution in a network context can be broadly classified into two categories: dynamics *of* networks, and dynamics *on* networks. The former refers to problems where the network structure itself changes over time according to some pre-specified rules of evolution; the latter refers to problems where there is a static network structure and the states of the nodes (variables associated with the nodes) evolve following pre-specified rules. These two categories are not mutually exclusive: one can model systems where both the nodal states and the network structure change over time (the term "adaptive networks" has been used for this combination, [13]).

In this work, we are interested in studying dynamics *on* networks at a coarse-grained level using a systematic model reduction framework called the *Equation-Free* approach [1, 15]. In this approach, short bursts of simulation at the ("fine") level of nodes and edges using the detailed rules of dynamic evolution of the problem are performed in order to estimate enough information to carry out computational tasks at a more coarse-grained level. The Equation-Free approach has been, in the past, successfully implemented for a variety of specific network models [16, 17, 18]. The success of this approach rests heavily on (a) defining a suitable set of coarse observables in terms of which a closed, reduced description of the evolution on the network may theoretically be obtained, and (b) the ability to convert back and forth between the two levels of description of the system - the "fine" and the "coarse-grained" levels. Thus, one of the most important steps in coarse graining using this approach is the selection of appropriate coarse variables.

We propose a useful (and hopefully efficient) representation of coarse variables specifically for models describing dynamics *on* networks, when the states of the nodes of the network *quickly* become correlated with features of the nodes imparted by the network, such as the node degree and/or the node clustering coefficient. In such cases we show that one can expand the function representing the dependence of node state to node structural identity in terms of suitable orthogonal polynomials depending on the distribution from which the node feature(s) is sampled (i.e. depending on the topology of the underlying network). This idea is analogous to the study of the effects of random parameters with

a known distribution on uncertain dynamical systems [19], and we will discuss this analogy in more detail below.

In order to illustrate these ideas we consider a simple agent-based model of opinion propagation where the agents are connected by a social network; simulations of this model indicate that the states of the agents become quickly correlated to the connectivity degrees of these agents as nodes in the network. The paper is organized as follows: Our illustrative model is described in Sec. 2, along with a quick overview of its nonlinear dynamic behavior. Sec. 3 defines and describes the coarse representation that forms the basis of our computational reduced model. A few details of the coarse variable description are relegated to the Appendix, in order to maintain the simplicity and flow of the discussion. A brief outline of the Equation-Free approach employed to computationally implement the reduced model is described in Sec. 4, along with the results of Equation-Free computations. In Sec. 5, we summarize the results and briefly discuss possible extensions and directions for future work.

2. The Model

We consider a simple, illustrative model of information propagation in a population of agents connected by a social network structure, as described in [20]. We briefly describe the individual-based rules of evolution of the model, that is, the dynamics at the level of agents/nodes and connections between them. We consider a population of N agents (numbered from 1 to N) connected in a network G with corresponding adjacency matrix A (i.e., if agents i and j are connected to each other, $A(i, j)$ is 1; if not, $A(i, j) = 0$). Each agent i is associated with a single scalar variable X_i, that denotes the emotional state of the agent. The variables X_i are bounded between -1 and 1. The agents receive "public information" at discrete time instances from the external environment; the information arrival times are modeled as a Poisson process. In addition to this public information, the agents also receive "private information" from their social environment (from their immediate neighbors in the social network). The emotional state of each agent changes according to the following rules:

1. The emotional state of each agent decays exponentially in time to zero. Thus, if Δt is the time interval between two consecutive arrivals of information, the emotional state of every agent decreases by a factor of $exp(-\gamma \Delta t)$ in this time interval, where γ is the decay parameter.

2. Public information is classified as "good" or "bad", both modeled as Poisson processes with arrival rates ν^+ and ν^- respectively. Whenever agents receive good (respectively, bad) public information, their emotional state jumps by a small, finite positive constant (resp., negative) value ϵ^+ (resp., ϵ^-).

3. The occurrence of private information transfer through the social network is also modeled as a Poisson process, similar to public information arrivals; but private information arrival rates are taken to be proportional to the connectivity degree of the receiving agent. Hence, the time interval
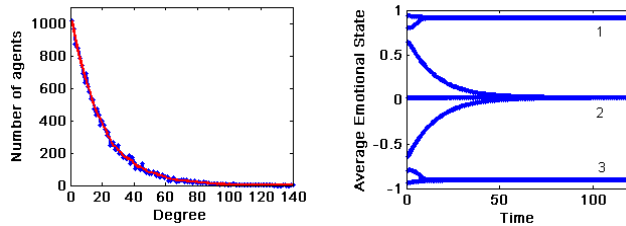
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Figure 1: **Left:** The degree histogram of the illustrative network structure (i.e., the number of agents with a given degree plotted versus the degree) used in numerical simulations is plotted as (blue) dots. The theoretical degree histogram from which our particular degree sequence is sampled is plotted as a (red) solid line. **Right:** Evolution in time of the average emotional state of all the agents in the network for the parameter settings listed in the text. Depending on the initial conditions, the system reaches one of three stable steady states (marked 1, 2 and 3).

between arrivals of private information for agent i with degree d_i is modeled as a Poisson process with mean αd_i where α is a positive constant. Whenever an agent is due to receive private information he/she compares his/her state with the state of an immediate neighbor, chosen at random. If the emotional state of this neighbor is larger (resp., smaller) than the emotional state of the agent, then a constant parameter e^+ (resp., e^-) is added to the agent's emotional state. Note that e^+ and e^- are positive and negative respectively.

4. In order to ensure that the emotional states stay within the lower and upper bounds of -1 and 1, whenever the emotional state of an agent reaches these bounds, the state is locked to that value for the remaining fragment of the time interval, regardless of the arrival of new information. This can be thought of as a saturation event where the agent finalizes his/her decision.

We used $N = 20,000$ agents in the model, and the network was constructed so that the degree distribution is a modified form of the discrete geometric distribution with degrees up to an upper limit of 140. The parameter p of this truncated geometric degree distribution is taken to be 0.05. The degree histogram for the network structure that we use for numerical simulations is plotted as (blue) dots in the left plot of Fig. 1. The theoretical histogram corresponding to the truncated degree distribution is plotted as a (red) curve for comparison. The following values were used for the remaining parameters of the model for the purpose of numerical simulations: $\nu^+ = 20; \nu^- = 20; \epsilon^+ = 0.075; \epsilon^- = -0.072; e^+ = 0.033; e^- = -0.035; \alpha = 2; \gamma = 0.5$. Of course, it would be interesting to investigate the effects of systematically varying these parameters, but we do not address that question here.
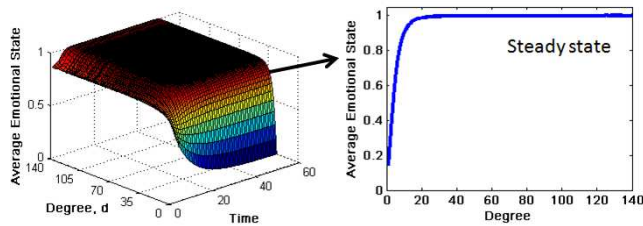
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Figure 2: A $3D$ plot of the evolution of the average emotional state of agents with a given degree versus the degree is shown evolving over time on the left. The steady state of this average emotional state versus degree is shown on the right. The initial condition for the simulation gave all agents a uniform emotional state of 0.8.

2.1. Nonlinear model behavior

The dynamical behavior of the model is described in considerable detail in [20]. We briefly recount some basic features of these dynamics here. Direct simulations, using the model rules, initialized at different initial conditions are presented. The state of the system at any moment in time is completely specified by the states of each of the $20,000$ agents in the network. Certain properties of the system can be best conveyed through chosen collective observables that are hopefully representative of the overall dynamics of the system. The average emotional state of all network agents is one such observable of interest. The evolution of average emotional state of all the agents in the network from various distinct initializations is shown in Fig. 1; for simplicity, the states of all the agents were initialized uniformly at fixed values over the network (but different fixed values for each initialization). The figure shows that the system reaches one of three stable steady states depending on the initial conditions; parameter settings leading to a single stable, or to two stable stationary states also exist in a detailed bifurcation diagram and have been discussed in [20].

3. Coarse representation

To obtain a reduced model, one must first select a set of coarse variables that accurately capture the long-term evolution of the system. To motivate our choice, we examined the detailed profiles of system states along an ensemble of trajectories like the ones summarized in Fig. 1. For this model, we observed that the states of the agents *quickly become highly correlated* with their degrees. Fig. 2 shows the evolution in time of the average state of all agents in a degree class (i.e., all agents having the same degree) as a function of the degree. The curve evolves smoothly in time, and it was demonstrated in [20] that such a correlation could indeed be used to obtain a reduced description of the model. A method of "binning" was employed in that work to construct good collective variables: this involved partitioning the network nodes into different groups

(based on the node degrees) and required 80 such groups, leading to 80 coarse variables.

We now realize that what, in that paper, was an *ad hoc* reduction is just a special case of a very general, and potentially powerful approach to systematically reducing the dynamics of large/complex networks. Instead of following the behavior of each agent, we *exploit* the (assumed) fact that structurally similar agents have similar behavior and can be tracked together. We assume here that the key variable that describes structural similarity is *the degree* of the agent in the network. The extension to more identities encompassing more structural features, and to possibly *intrinsic* heterogeneities between the agents, over and beyond the network-imparted *structural* heterogeneities will be addressed in our Discussion section. Finding the relationship between agent structural characteristics (here, agent degrees) and agent states generates a coarse description, whereby the system state can be encoded in (hopefully drastically) fewer independent variables. Previous work coarse-graining in terms of network properties has used the graph Laplacian [16], and we have previously used expansions in terms of *intrinsic* heterogeneities [29, 18].

Let x_d denote the average emotional state of all agents with degree d, where $d \in [1, 140]$. Then, the curve in Fig. 2 can be represented by a function $x_d = f(d)$. Note that since the degrees of the nodes in the network range between 1 and 140, this "curve" is, in effect, a vector of 140 values. An intuitive approach to obtaining a reduced description of the function f is to expand it in terms of suitable basis functions. Consider, for example, some set of orthogonal polynomials p_i as basis functions, where $i \in [1, k]$. One can then expand the function f in terms of these basis functions as

$$f(d) = \sum_{i=1}^{k} c_i p_i(d). \tag{1}$$

If the k basis functions suffice to accurately capture the shape of the function, one can then use the k coefficients c_i as the coarse representation of $f(d)$. Once the polynomials are selected, the common method to evaluate the coefficients is to find the optimal values of these coefficients that minimize the residual defined below:

$$\left\langle f(d) - \sum_{i=1}^{k} c_i p_i(d), f(d) - \sum_{i=1}^{k} c_i p_i(d) \right\rangle_{w(d)}. \tag{2}$$

Note that the inner product in the residual is defined with respect to a weight function $w(d)$. In our example, the values of the function $f(d)$ which describes the average state for every degree class is computed *using different numbers of agents at each d*. It is therefore reasonable to use a weight function which mirrors this sampling. In simple terms, if there are many agents with a given degree d, the average emotional state of agents in that degree class is calculated with more fidelity; more weight should be given to the corresponding degree class, so that the value corresponding to the degree class is given more importance
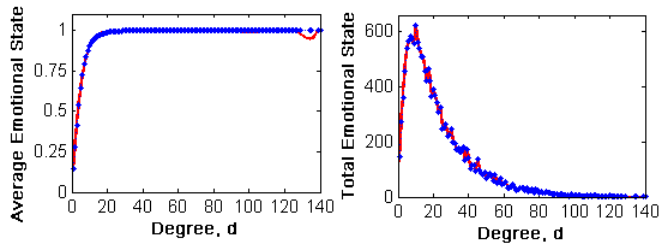
Figure 3: **Left:** The steady state average emotional state of all the agents with a specified degree (as in the right plot of Fig. 2) is plotted versus the degree as (blue) dots. The curve fit obtained by using 10 of our orthogonal polynomials is plotted as a (red) solid curve for comparison. **Right:** For the same case, the *total* emotional state of all the agents with a specified degree is plotted versus the degree as (blue) dots. This plot on the right is just a product of the plot on the left and the degree histogram shown in Fig. 1. The (red) solid lines correspond to the results from our polynomial approximation procedure.

in the approximation procedure. We choose simple proportional weights which implies $w(d) = h(d)$, where $h(d)$ represents the histogram of degrees (i.e., $h(d)$ is the number of agents in the network with degree d).

The polynomials p_i are thus chosen to be orthogonal with respect to the degree distribution $h(d) = w(d)$. This orthogonality condition can be described as follows:

$$\langle p_i(d), p_j(d) \rangle_{w(d)} = \delta_{ij}. \tag{3}$$

Since the polynomials are orthogonal with respect to the weight distribution, the coefficients that minimize the residual (with respect to the same weights) in Eq. 2 can be directly evaluated by the following simple expression:

$$c_i = \langle p_i(d), f(d) \rangle_{w(d)}. \tag{4}$$

What remains to be discussed is the selection of suitable polynomials. For this portion, we borrow tools developed in the context of uncertainty quantification in dynamical systems with random parameters. In such problems, the effect of a random parameter (e.g. normally distributed) on the system state can be represented through orthogonal polynomial expansions in terms of appropriate random variables [19]. These orthogonal polynomials are termed "polynomial chaos" (PC), and projections of the system states onto the Polynomial Chaos (PC) coefficients evolve deterministically in time. Such polynomials were initially proposed for Gaussian random parameters, but a generalized approach for other random parameter probability measures based on the Askey scheme was developed in [21]. These generalized polynomials, the "Wiener-Askey polynomial chaos", are constructed so that they are orthogonal with respect to a variety of known probability distributions. In our case, the random parameter of interest *is the degree distribution itself*, and it is a *truncated* geometric distribution. If we approximate this as a (continuous) geometric distribution, the Wiener-Askey

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scheme suggests Meixner polynomials as basis functions. The derivation of orthogonal polynomials for any (discrete, possibly truncated/empirical) weight function $w(d)$ (which we used for our numerical computations) is discussed in the Appendix.

In Fig. 3, we re-plot the curve of average emotional state versus degree at the "top" steady state branch (steady state 1 in Fig. 1) using (blue) dots. We evaluate the first 10 polynomials that are orthogonal to the degree distribution of our particular network, sampled empirically from the "theoretical" truncated geometric distribution. The corresponding 10 coefficients are evaluated using Eq. 4 and our approximation of the system state $f(d)$ is then reconstructed using Eq. 1 with $k = 10$. This reconstructed curve is plotted as a (red) continuous line in the same figure, for comparison to the original curve. Notice that the fit is more accurate at lower degree values, compared to that at higher values; this is due to the small probability of high degrees - in other words, due to the weight function used in our approximation procedure. As can be seen in the left plot of Fig 1, the degree histogram is heavily concentrated at lower degrees, and hence the states corresponding to these degrees are better approximated in the reduction/reconstruction. When we plot the *total* emotional state of a given degree class (the sum of the emotional states of all the agents with the same degree) versus the degree, as shown on the right side of Fig. 3, the error associated with our reduction/approximation procedure is clearly much more uniformly spread across the degree classes.

4. Coarse modeling and computational results

Once the coarse variables of the model have been defined, the Equation-Free approach [1, 15] can be used to computationally implement the coarse model. The Equation-Free (EF) approach to modeling/computation is a framework that has been developed for problems that can, in principle, be described at multiple -here, two- levels. The evolution equations are available at a "fine", microscopic scale (here at the level of individual nodes/agents and edges/connections) while the equations for the "coarse", macroscopic behavior (here, a handful of expansion coefficients for the function $f(d)$) are not available in an explicit, closed form. In this approach, short bursts of simulations at the "microscopic" node level are used to estimate information such as time-derivatives, or actions of Jacobians, pertaining to the coarse variables. This is accomplished through the definition of operators that allow us to "translate" between coarse variables and consistent detailed, fine variables. The transformation from coarse to fine variables is called the *lifting* operator (L), while the reverse transformation is called the *restriction* operator (R).

In our example, the fine variables of the model are the individual states of all the agents in the social network, while the coarse variables are the coefficients c_i referred to in Sec. 3. The microscopic rules of evolution defined in Sec. 2 constitute the detailed, microscopic time-evolution operator defined by ϕ_t (where t represents the number of time steps or iterations). The macroscopic evolution

operator can then be defined in terms of this microscopic evolution operator as well as the lifting and restriction operators as follows:

$$\Phi_t(\cdot) = R \circ \phi_t \circ L(\cdot). \tag{5}$$

In other words, the evolution of the coarse variables can be represented as:

$$\mathbf{c}(T + t) = \Phi_t(\mathbf{c}(T)),$$

where Φ_t is defined in Eq. 5 and $\mathbf{c}$ represents the vector of coefficients $[c_1, c_2,... c_k]$.

We will illustrate the EF approach by describing two particular algorithms: *coarse projective integration* [22, 23] and coarse fixed point computation [24]. In coarse projective integration, the detailed system is integrated forward in time using short bursts of fine-scale, microscopic simulations, and the results are used to estimate time derivatives of the coarse variables, which are then used to project these latter variables forward in time. Starting from a specified initial condition in terms of the "microscopic" variables (the emotional states of the agents), the following steps are carried out to implement coarse projective integration:

1. **Simulation**: The detailed model is run for a specified period of time, say 10 time steps (to be exact, 1000 sample realizations are run and averaged).

2. **Restriction**: The coarse variables are evaluated at each time-step of the simulation. For our example, this involves computing the coefficients c_i given in Eq. 4.

3. **Projection**: The last few observations of the coarse variables c_i from the previous step are used to estimate their time-derivative. The coefficients are then projected forward in time over another 10 time steps using a simple linear extrapolation. Consider a standard differential equation $dx/dt = f(x)$. The forward Euler scheme would read

$$x(t + \Delta t) \approx x(t) + \Delta t f(x(t)).$$

Our projection is similar to this, except the time derivative ($f(x(t))$ above) does not come from a closed formula ($f(x)$), but is instead estimated from the computational observations of the fine scale model.

4. **Lifting**: Since estimates of the coarse variables c_i are available at the projected time, we have to transform them to a consistent set of agent states for all the agents before the fine scale model can evolve again. This can be achieved by expanding the polynomials according to Eq. 1. Once the states of all the agents in the network are computed, they can be used as the initial condition to restart simulations as given in Step 1. Note that, if any of the agent states lie outside the acceptable range of values (above 1 or below -1), the states are revised to the limiting values (1 and -1 respectively).

These steps, performed repeatedly, constitute coarse projective integration, which is used to accelerate computations in systems with separations of time scales. In our illustrative EF computations, we retained all model parameter values mentioned above; for the coarse representation we used 10 polynomials, constructed to be orthogonal to our network's degree distribution. Using the corresponding 10 coefficients as coarse variables, we implemented coarse projective integration for the trajectory shown in Fig. 2. The evolution of the 10 coefficients are shown as solid lines in Fig. 4. The first 5 coefficients are shown on the left and the next 5 are shown on the right. The results of coarse projective integration, where fine scale simulations are carried out for only half of the computed trajectory (leading to a factor of two in acceleration) are shown as dots for comparison in the same figure. It can be seen that the coarse evolution can be captured well by our implementation of the reduced model.

In addition to accelerating simulations, we can use the Equation-Free framework to also quickly find coarse steady states (corresponding to stationary states of the detailed, stochastically evolving model). This is done using a coarse fixed point solver: to compute the steady states values of the coefficients $\mathbf{c}$, we have to solve the following equation:

$$F(\mathbf{c}) := \mathbf{c} - \Phi_{10}(\mathbf{c}) = 0, \tag{6}$$

where Φ_t is the coarse time-stepper over t time steps. The roots of F can be found using a damped Newton-Krylov GMRES iteration scheme [25, 26]. In the standard Newton-Raphson algorithm, the value of $\mathbf{c}$ would be updated by the equation

$$\mathbf{c}_{n+1} = \mathbf{c}_n + \Delta\mathbf{c}, \tag{7}$$

where $\Delta\mathbf{c}$ is found as the solution to

$$[DF(\mathbf{c}_n)]\Delta\mathbf{c} = -F(\mathbf{c}_n). \tag{8}$$

The action of the Jacobian $DF(\mathbf{c}_n)$ can be estimated indirectly (since an analytical expression would require analytically differentiating the coarse time-stepper $\Phi_t(\mathbf{c})$ in Eq. 6) using the coarse time stepper. We use a Krylov-based approach where the action of this Jacobian on known vectors, its matrix-vector products, is required to solve the equation; this Jacobian can be estimated through numerical differentiation (i.e., evaluating the coarse time-stepper at appropriately selected perturbations of the $\mathbf{c}$ values). Such iterative *matrix-free* computations are naturally suitable for Equation-Free computation, where explicit Jacobians are not available in closed form.

The results of coarse fixed point computations are shown in Fig. 5. The first two plots in this figure show the actual steady state (resp., the *average* and *total* emotional state of agents with a given degree plotted against the degree class) computed using direct simulations as (red) dots. The coarse steady state computed using the procedure described in the previous section is plotted as a solid blue line. The convergence of the norm of F as defined in Eq. 6 is shown on the right plot of the same figure.
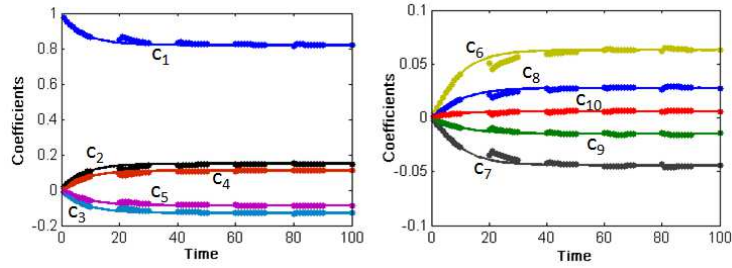
Figure 4: Evolution of the coarse variables corresponding to Fig. 2. The solid lines indicate results obtained from direct simulations. The dots indicate results obtained through coarse projective integration using 10 coefficients (accelerating the overall simulation by a factor of 2) The plot on the left shows the evolution of the first 5 coefficients, while the plot on the right shows that of the next 5 coefficients.
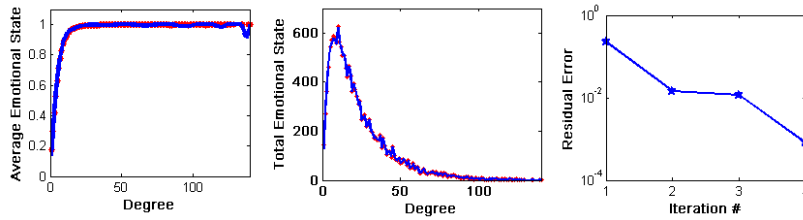

Figure 5: **Left:** The steady state *average* emotional state of agents of a specified degree versus the degree is plotted as (red) dots. The lifting of the coarse steady state computed by Newton-GMRES algorithm is plotted as a (blue) solid curve. **Center:** The steady state *total* emotional state of agents of a specified degree versus the degree is plotted as (red) dots. The lifting of the coarse steady state computed by Newton-GMRES algorithm is plotted as a (blue) solid curve. **Right:** Convergence of Newton-GMRES: The L_2 norm of the coarse residual is plotted against the iteration number. Computations were performed with a 10 polynomial coarse basis.
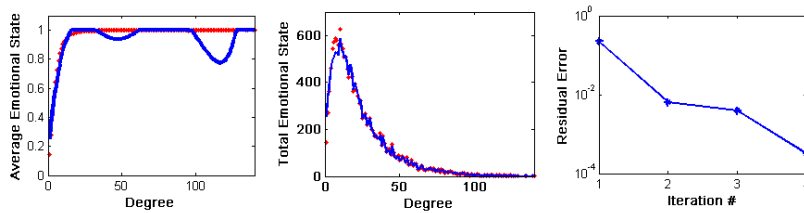
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Figure 6: **Left:** The steady state *average* emotional state of agents of a specified degree versus the degree is plotted as (red) dots. The lifting of the coarse steady state computed by Newton-GMRES algorithm is plotted as a (blue) solid curve. **Center:** The steady state *total* emotional state of agents of a specified degree versus the degree is plotted as (red) dots. The lifting of the coarse steady state computed by Newton-GMRES algorithm is plotted as a (blue) solid curve. **Right:** Convergence of Newton-GMRES: The L_2 norm of the coarse residual is plotted against the iteration number. Computations were performed with a 6 polynomial coarse basis.

It is important to note here that although we need 10 coefficients to get a visually acceptable fit for the curve of average emotional state versus degree, we can use an even smaller number of coefficients for an even more parsimonious coarse-graining. For instance, in Fig. 6, we show the results of coarse fixed point computations through Newton-GMRES using just 6 polynomials. The plots in the figure are similar to the ones shown in Fig. 5. Although the polynomial fit truncated at 6 coefficients deviates visibly from the steady state function value, especially at higher degrees (for reasons mentioned earlier), (a) the plot on the right shows that the procedure with 6 coarse variables does converge, and (b) the actual steady state can be easily recovered by running simulations for a very short time from the lifting of the computed coarse steady state. Instead of truncating (setting higher order polynomial coefficients in the reconstruction to zero), "slaving" these coefficients to the lower ones -in effect, constructing a six-dimensional "slow manifold" for the process dynamics- will provide even more accurate/more reduced models.

5. Discussion

In this work we discussed a systematic approach to coarse graining dynamics of coupled networks of units (nodes, agents), and demonstrated its application through the illustrative computational coarse-graining of an agent-based model with an underlying network structure. In this model, the state of the agents was observed to quickly become highly correlated with the degree of the agents; our coarse graining methodology takes advantage of this fact in constructing a set of appropriate collective variables. The resulting reduced model was computationally implemented using the Equation-Free approach.

In the selection of our collective variables we took advantage of concepts developed in the context of Uncertainty Quantification for studying the effect of a random parameter in differential equations; in effect, we are performing

"Heterogeneity Quantification" rather than Uncertainty Quantification. In UQ problems, the effect of a *random* parameter with a known distribution on the system state is captured by expanding the state in terms of orthogonal polynomials of the random variables. The orthogonal polynomials used depend on the distribution from which the random variables are sampled. In our case, the states of the agents depend on the agent structural identities (here, agent degrees, whose distribution is prescribed by the network) -and, of course, on time. By analogy, we can think of the degrees as a "random heterogeneity parameter" with a given distribution, and parsimoniously capture its effect on the agent states by expanding the states in terms of suitable orthogonal functions of the degree. It is clear that the approach can be extended to states that depend on "higher order" structural identities - identities that do not only depend on the degree, but also on more/different network statistics: for example, degree *and* clustering coefficients for each node. The joint distribution of these latter two features will again be dictated by the network, and the basis functions will be now two-dimensional - clearly, the integrals involved in computing the corresponding coefficients will start becoming cumbersome as the number of "determining features" grows. For such problems, there has already been considerable progress on collocation-based computations, and the use of sparse grids in the UQ literature [27, 28, 29] and we expect that these tools will also become useful in network coarse-graining when multiple network features affect the system state. Still, there is no reason for the roots of polynomials orthogonal with a given degree distribution weight to be themselves integers, and so collocation approaches to approximating integrals over degree distributions must be addressed.

We demonstrated how to computationally take advantage of a coarse model through coarse projective integration and coarse fixed point computations. It is well known, and reasonably straightforward to extend the EF approach to other system-level computational tasks, such as coarse bifurcation analysis, coarse stability analysis etc. as reviewed in [15]. It is also worth mentioning that the approach described here is in principle broadly applicable to coarse-graining other dynamical problems consisting of heterogeneous coupled units. Here the relevant heterogeneity was the number of connections for each node (its degree); in other network problems the heterogeneity may involve a non-network feature (an "intrinsic feature) of the node (e.g., age or fitness of a node), or even possibly joint distributions of "network (structural)" and "non-network (intrinsic)" heterogeneity features. We are currently working on such "joint heterogeneity quantification" problems.

We conclude by mentioning an additional, possibly important, consideration. In recent literature on coupled oscillators (an area where our approach can also be exploited) mean-field theories have been developed, expressing the behavior of the network (the statistics of the distribution of oscillator angles) as a function of the network degree [14]. What is of particular interest in our discussion is that, in order to derive explicit mean field equations for behavior as a function of degree, the authors could also include additional structure in the form of a prescribed "degree assortativity", the probability that a node with degree k_i is

connected with a node of degree k_j; they also considered the case of *no* assortativity. In our case, we do not derive such equations explicitly, but we solve them through our equation-free approach. All our computations above were performed with a fixed, static network, with a particular, prescribed degree distribution; choosing that particular network, also *de facto* selected all additional high order statistics through the network construction (including a particular assortativity). In that sense, our equations constitute a coarse-graining *of the particular network*.

It is also conceivable that one may want to construct (and average over) several sample networks *with the same statistics*, here the same degree distribution (see, e.g., the discussion in [30]). Then the equation-free approach does not solve for a coarse-graining of a particular realization, but rather for the *expected* behavior over realizations with a prescribed degree distribution. Creating several such network samples will be used to estimate the common degree distribution needed to compute our orthogonal polynomial basis. It is thus our *lifting step* that determines what coarse-grained problem we are solving. Lifting to always the same network (resp. lifting to networks with prescribed degree distributions only (and averaging over them), resp. lifting to networks with prescribed degrees and assortativities (and averaging over them)) yields different coarse-grained problems. Our approach can be used to tackle all these problems (and obvious variations/extensions of them) by judiciously selecting what subset of realizations is constructed in the lifting step.

For our illustrations we focused on the identification of collective variables of detailed individual-based models evolving on networks whose statistical properties can be described by the degree distribution. The degree distribution is one of the most important features one would determine to assess the heterogeneity of the underlying structure. It suffices to characterize the statistical properties of uncorrelated networks such as ER [10, 9] and scale-free-like structures (under certain assumptions) (see for example [31, 32]). While this is usually one of the first statistical measures one would use to study the influence of the topology on the emergent dynamics, the proposed methodology can be epxloited as a basis for the investigation of more complex topologies. For example, for correlated structures such as small-world topologies and scale-free networks one should also take into account other distributed characteristics such as clustering, degree correlation (assortativity) and betweenness. In such cases, for the construction of consistent with these distributions networks one has to employ relevant algorithms for their at-will adjustment (see for example [34, 35, 36, 37]).

Finally, it is conceivable that the approach may be extended to encompass cases where not only the state of the nodes, but the statistics of the network itself may evolve over time - so that not only dynamics *on* networks -like here-, but *adaptive network* dynamics (dynamics simultaneously *on* and *of* networks) could be tackled.

a research visit to Princeton.

Appendix A. Finding a suitable basis of orthogonal polynomials tailored to a given degree distribution

The procedure that we use to evaluate a set of polynomials orthogonal to one another with respect to an empirical weight distribution [33] (defined over a range of integers, here the node degrees) is described here. Let the i-th required polynomial be denoted by p_i, and let $w(d)$ be the specified discrete weight distribution. p_i can be written using the following general representation:

$$p_i = \alpha_i \left(1 + \sum_{j=1}^{i-1} y_{ij} d \right). \tag{A.1}$$

The orthogonality condition is written as

$$\langle p_i, p_j \rangle_{w(d)} = \delta_{ij}. \tag{A.2}$$

Since we are interested in evaluating the function at discrete values of d, we may approximate the orthogonality condition by the following summation:

$$\sum_{d=1}^{140} p_i(d) p_j(d) w(d) = \delta_{ij}. \tag{A.3}$$

We are interested in finding the first k polynomials. This implies that we need to evaluate $k(k+1)/2$ polynomial coefficients, i.e., $k(k-1)/2$ for y_{ij}s and k for α_is. These can be *successively* evaluated by using the $k(k+1)/2$ orthogonality conditions: $k(k-1)/2$ for the case $i \neq j$ and k for the case $i = j$ respectively.

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