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Super compact pairwise model for SIS epidemic on heterogeneous networks

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In this paper, we provide the derivation of a super compact pairwise (PW) model with only four equations in the context of describing susceptible–infected–susceptible (*SIS*) epidemic dynamics on heterogenous networks. The super compact model is based on a new closure relation that involves not only the average degree but also the second and third moments of the degree distribution. Its derivation uses an *a priori* approximation of the degree distribution of susceptible nodes in terms of the degree distribution of the network. The new closure gives excellent agreement with heterogeneous PW models that contain significantly more differential equations.

Keywords: SIS epidemic; pairwise model; triple closure.

1. Introduction

While networks have provided a new modelling paradigm for population dynamics [1–3], these are still used in conjunction with mean-field models of various types. The most frequently used and well-known mean-field models for network epidemics are the degree-based mean-field model, also known as heterogeneous mean-field [3,4], and pairwise (PW) model [5–7]. Both continue to provide a productive framework for approximating expected values of random variables emerging from explicit network-based stochastic simulations in different contexts and networks with different properties. The major advantage of such mean-field models stems from the fact that often these allow us to analytically determine quantities such as the basic reproduction number, final epidemic size or endemic equilibrium [4,6]. Such analytic expressions then lead to a significantly better understanding of the interplay between network and disease characteristics.

PW models have originally been introduced in the context of mathematical ecology [8] followed by natural extensions to epidemiology [6]. The original simple model for undirected and unweighted networks has been subsequently extended to networks with heterogenous degree [9], directed networks [10], weighted networks [11], networks displaying motifs [12] and even combined with the edge-based compartmental modelling framework for an even more compact treatment [7].

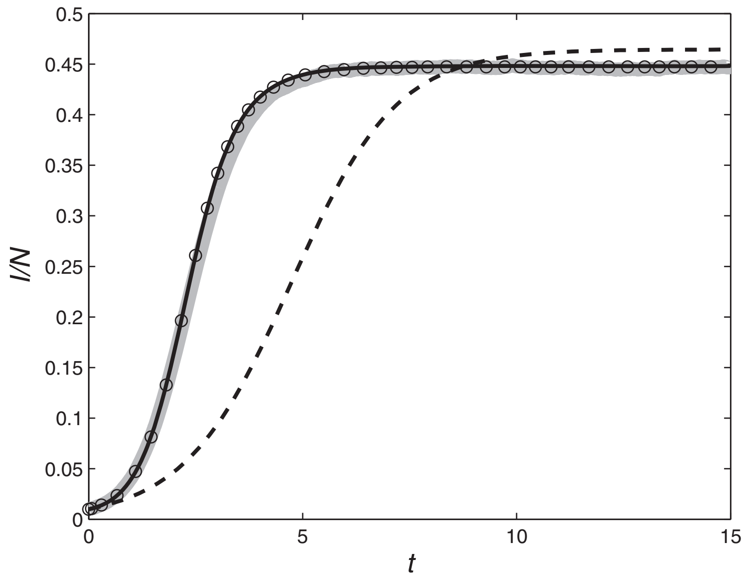

FIG. 1. SIS epidemic propagation on a bimodal configuration random graph: simulation (gray thick curve), PW (dashed), compact PW (continuous), heterogeneous PW (circles). The parameter values are $N = 1000$ nodes, half of nodes have degree $k_1 = 5$ while the other half have degree $k_2 = 35$. The recovery and per contact transmission rate are $\gamma = 1$ and $\tau = 3\gamma\langle k\rangle/\langle k^2\rangle$, respectively. The moments are defined as $\langle k^i\rangle = \sum k^i p(k)$, where $p(k)$ is the network's degree distribution.

The closure in the most basic or fundamental PW model is based on the assumption on homogeneity of the degree distribution, i.e. all nodes have approximately the same degree n. Hence, the conventional PW model cannot be applied for graphs with heterogeneous degree distribution, such as bimodal graphs or networks with power law degree distribution. This is shown in Fig. 1. For heterogeneous networks, a corresponding PW model was introduced in [9]. This gives excellent agreement with simulations for all configuration-like random networks [13], see Fig. 1. The heterogeneous PW model consist of order N^2 differential equations, where N denotes the number of nodes in the network. An approximation of pairs leads to a simpler system, called compact PW model that consist of only order N equations [7] and still gives very good agreement with simulations, see Fig. 1.

The aim of this paper is to introduce an even simpler model with only four equations that performs well for large heterogeneous networks. The system is derived from the compact PW model by introducing a further approximation, and using a closure relation that contains not only the average of the network's degree distribution but also its second and third moments.

2. Derivation of the super compact PW model

2.1 *PW model for homogenous networks*

We start from the exact PW model. For the *SIS* epidemic on an arbitrary undirected network, the expected values of $[S]$, $[I]$, $[SI]$, $[II]$ and $[SS]$ satisfy the following system of differential equations:

$$[\dot{S}] = \gamma[I] - \tau[SI], \tag{1}$$

$$[\dot{I}] = \tau[SI] - \gamma[I], \tag{2}$$

$$[\dot{SI}] = \gamma([II] - [SI]) + \tau([SSI] - [ISI] - [SI]), \tag{3}$$

$$[\dot{SS}] = 2\gamma[SI] - 2\tau[SSI], \tag{4}$$

$$[\dot{II}] = -2\gamma[II] + 2\tau([ISI] + [SI]), \tag{5}$$

where $[X]$, $[XY]$ and $[XYZ]$ denote the expected number of nodes in state X, edges in state $X-Y$ and triples in state $X-Y-Z$, respectively. For example, assuming the network at an arbitrary but fixed point in time, with all nodes labelled either S or I, the number of nodes in state S is simply $[S] = \sum_{i=1}^{N} S_i$, where S_i returns 1 if node i is susceptible and zero otherwise. Similarly, the number of $S-I$ links is $[SI] = \sum_{i=1}^{N} g_{ij} S_i I_j$, where the network is defined in terms of a symmetric adjacency matrix $G = (g_{ij})_{i,j=1,2,\dots,N}$ with no self-loops and with binary entries. As before, I_j returns 1 if node j is infected and zero otherwise. This effectively means that for undirected networks $[XY] = [YX]$, $[XX]$ is double the number of unique edges in state $X-X$, and similarly $X-Y-X$ accounts twice for a unique $X-Y-X$ triple, where $X, Y \in \{S, I\}$. The parameters τ and γ denote the per contact transmission and recovery rate, respectively. This system is derived directly from master equations in [14] and hence exact. We note that some of the equations can be omitted by exploiting conservation identities, such as $[S] + [I] = N$.

It is well known that in order to transform equations (1)–(5) into a self-consistent solvable system closures need to be applied in order to break dependency on higher order moments. Particularly useful are closures at the level of triples. As it is well known, the simplest closure is

$$[ASI] \approx \frac{n-1}{n}\frac{[AS][SI]}{[S]} = (n-1)[AS]\frac{[SI]}{n[S]}, \tag{6}$$

where $n = \langle k \rangle$ is the average degree of the network, and A stands for S or I. Intuitively, the closure means that the number of $A-S-I$ triples can be counted by considering all $(n-1)[AS]$ stubs emanating from S nodes which are already connected to a node in state A and multiplying this by the probability that such stubs will connect to an infectious node, i.e. $[SI]/n[S]$. This closure leads to the traditional PW system

$$[\dot{S}]_p = \gamma[I]_p - \tau[SI]_p, \tag{7}$$

$$[\dot{I}]_p = \tau[SI]_p - \gamma[I]_p, \tag{8}$$

$$[\dot{SI}]_p = \gamma([II]_p - [SI]_p) + \tau\frac{n-1}{n}\frac{[SI]_p([SS]_p - [SI]_p)}{[S]_p} - \tau[SI]_p, \tag{9}$$

$$[\dot{SS}]_p = 2\gamma[SI]_p - 2\tau\frac{n-1}{n}\frac{[SI]_p[SS]_p}{[S]_p}, \tag{10}$$

$$[\dot{II}]_p = -2\gamma[II]_p + 2\tau\frac{n-1}{n}\frac{[SI]_p^2}{[S]_p} + 2\tau[SI]_p. \tag{11}$$

Here the subscript p is used to emphasize that the solution of this system is different from the exact values of the expected variables. As Fig. 1 shows, this system cannot capture network heterogeneities, hence closure (6) needs improvement.

2.2 *PW models for heterogenous networks*: *the heterogeneous*, *pre-compact and compact PW models*

The problem with closure (6) is that it assumes that each node has degree n, which is obviously a crude approximation for heterogeneous networks. This has led to several heterogeneous mean-field models, where the state space is much extended to account for the expected number of nodes in different states and with a given degree, i.e. $[S_k](t)$ and $[I_k](t)$ for the expected number of susceptible and infected nodes of degree k, respectively. These new variables will induce or require further variables at pair level, such as $[S_kI_l](t)$ which denotes the expected value of the number of edges connecting susceptible nodes of degree k to infected nodes of degree l. In this spirit, the following heterogeneous models were developed in historical order:

- heterogeneous PW model [9],
- pre-compact PW model [9] and
- compact PW model [7].

Instead of presenting the systems of differential equations of these models and working from the most explicit or complex to the more compact one, we start from the simplest model and show in an intuitive way how the more sophisticated models arise. Since closure (6) uses the degree of the middle node, it is useful to express the triple as

$$[ASI] = \sum_{k=1}^{K} [AS_kI],$$

where the different degrees occurring in the graph are $k = 1, 2, \ldots, K$. The closure for the triples in the right-hand side can be written as

$$[AS_kI] \approx \frac{k-1}{k} \frac{[AS_k][S_kI]}{[S_k]}. \tag{12}$$

In order to use this closure in the exact system (1)–(5), one needs differential equations for $[S_k]$, for $[S_kI]$ and for $[S_kS]$. The exact differential equations for $[S_k]$ are

$$[\dot{S_k}] = \gamma[I_k] - \tau[S_kI], \quad k = 1, 2, \ldots, K, \tag{13}$$

where the substitution $[I_k] = N_k - [S_k]$ can be used. The simplest heterogeneous model [7] uses only $[S_k]$ as new variables and introduces an algebraic expression that approximates $[S_kI]$ and $[S_kS]$ in terms of $[S_k]$, $[SI]$ and $[SS]$ as follows:

$$[S_kI] \approx [SI] \frac{k[S_k]}{\sum_{l=1}^{K} l[S_l]}, \tag{14}$$

which can be interpreted as showing that the ratio of the number of edges connecting degree k susceptible nodes to infected nodes and the number of SI edges is almost the same as the ratio of the number of stubs starting from degree k susceptible nodes and the total number of stubs starting from susceptible nodes. Using this approximation, closure (12) can be simplified as given below

$$[AS_kI] \approx \frac{k-1}{k} \frac{[AS_k][S_kI]}{[S_k]} \approx \frac{k-1}{k} \frac{[AS][SI]k^2[S_k]}{S_1^2} = \frac{[AS][SI]k(k-1)[S_k]}{S_1^2}, \tag{15}$$

where $S_1 = \sum_{k=1}^{N} k[S_k]$ is the first moment of the distribution of susceptible nodes. This leads to the so-called compact PW model, in which the variables are: $[SI]$, $[SS]$, $[II]$ and $[S_k]$ for $k = 1, 2, \ldots, K$, i.e. it contains $K + 3$ differential equations. In fact, the system consists of equations (13), and (3)–(5) with the above-mentioned closures and approximations, namely (14) and (15). Thus, it takes the form

$$\dot{[S_k]}_c = \gamma [I_k]_c - \tau k [S_k]_c \frac{[SI]_c}{S_s}, \tag{16}$$

$$\dot{[I_k]}_c = \tau k [S_k]_c \frac{[SI]_c}{S_s} - \gamma [I_k]_c, \tag{17}$$

$$\dot{[SI]}_c = \gamma([II]_c - [SI]_c) + \tau([SS]_c - [SI]_c)[SI]_c P - \tau [SI]_c, \tag{18}$$

$$\dot{[SS]}_c = 2\gamma [SI]_c - 2\tau [SS]_c [SI]_c P, \tag{19}$$

$$\dot{[II]}_c = 2\tau [SI]_c - 2\gamma [II]_c + 2\tau [SI]_c^2 P, \tag{20}$$

$$S_s = \sum_{k=1}^{K} k[S_k]_c, \quad P = \frac{1}{S_s^2} \sum_{k=1}^{K} (k-1)k[S_k]_c. \tag{21}$$

Here the subscript c, referring to the word 'compact', is used to emphasize that the solution of this system is different from the exact expected values.

The next level of complexity is represented by the pre-compact PW model, in which the variables $[S_k I]$ and $[S_k S]$ are kept as independent variables and differential equations for these are written down. Thus, the systems can be formulated in terms of variables, such as $[S_k]$, $[S_k S]$, $[S_k I]$, $[I_k S]$ and $[I_k I]$, i.e. resulting in a total of $5K$ variables. This can be done by considering the closure introduced in [9] which is

$$[A_n B_m] = \frac{[A_n B][A_n B]}{[AB]} \frac{[N_n N_m] \sum_q q[N_q]}{n[N_n] m[N_m]}, \tag{22}$$

where N_k denotes the number of nodes of degree k. It is worth noting that this system is not able to account for preferential mixing.

The most complex system, which we call heterogeneous PW model, uses all combinations of pairs as variables, namely $[S_k S_l]$, $[S_k I_l]$ and $[I_k I_l]$. Hence, it consists of $2K^2$ differential equations. At the price of having a system with the number of equations of quadratic order, we do not need any extra approximations (besides the closures), such as (14) in the compact PW model, or (22) for the pre-compact PW model. Without explicitly including the closures, the most complex system can be written as

$$\dot{[S_k]} = -\tau \sum l[S_k I_l] + \gamma [I_k], \tag{23}$$

$$\dot{[I_k]} = +\tau \sum l[S_k I_l] - \gamma [I_k], \tag{24}$$

$$\dot{[S_k S_l]} = -\tau \sum_m ([I_m S_k S_l] + [S_k S_l I_m]) + \gamma([S_k I_l] + [I_k S_l]), \tag{25}$$

$$[\dot{S_kI_l}] = +\tau\sum_m([S_kS_lI_m] - [I_mS_kI_l]) - (\tau+\gamma)[S_kI_l] + \gamma[I_kI_l], \tag{26}$$

$$[\dot{I_kI_l}] = +\tau\sum_m([I_mS_kI_l] + [I_kS_lI_m]) + \tau([S_kI_l] + [I_kS_l]) - 2\gamma[I_kI_l], \tag{27}$$

with all subscripts going from $1, 2, \dots, K$.

2.3 *Super compact PW model with heterogeneous triple closure*

We now show that the network heterogeneity can be captured by a small system, containing only four differential equations, just as in the simplest PW model. Consider a random network with degrees $d_1, d_2, \dots, d_K$ and denote the number of nodes of degree d_k by N_k for $k = 1, 2, \dots, K$, i.e. $N_1 + N_2 + \cdots + N_K = N$. We point out that denoting degrees as d_k instead of k will prove to be advantageous in the derivation below. The degree distribution of the graph is then given by $p_k = N_k/N$. The average degree and the second moment of the degree distribution are

$$\langle k\rangle = \frac{1}{N}\sum_{k=1}^{K} d_kN_k, \quad \langle k^2\rangle = \frac{1}{N}\sum_{k=1}^{K} d_k^2N_k. \tag{28}$$

In order to arrive to our new even more simplified system, the super compact PW model, we start from a triple and the closure given in (15)

$$[ASI] = \sum_{k=1}^{N}[AS_kI] \approx \frac{[AS][SI]}{S_1^2}\sum_{k=1}^{N} d_k(d_k-1)[S_k] = [AS][SI]\frac{S_2 - S_1}{S_1^2},$$

where we used closures (12) and (14), and where $S_2 = \sum_{k=1}^{K} d_k^2[S_k]$ is the second moment of the distribution of susceptible nodes. Thus, in order to use this closure in the exact system (1)–(5) one needs an algebraic expression of S_2 and S_1 in terms of variables $[S]$, $[I]$, $[SI]$, $[II]$ and $[SS]$ only. Expressing the total number of stubs starting from susceptible nodes we get $S_1 = [SI] + [SS]$ as an exact relation. Thus, the problem arises from the fact that such an exact relation is not available for the second moment S_2. Our heuristic idea to obtain a good approximation of $(S_2 - S_1)/S_1^2$ is the following. Dividing the equation $[S] = \sum_{k=1}^{K}[S_k]$ by $[S]$, we get that $[S_k]/[S]$ is a probability distribution. The expected value of this distribution is known, it is

$$\sum_{k=1}^{K} d_k\frac{[S_k]}{[S]} = n_S := \frac{[SI] + [SS]}{[S]},$$

or in other words the average degree of susceptible nodes. Our idea is to use an *a priori* approximating distribution for $[S_k]/[S]$ that will be denoted by s_k. This approximating distribution satisfies

$$s_1 + s_2 + \cdots + s_K = 1, \tag{29}$$

$$d_1s_1 + d_2s_2 + \cdots + d_Ks_K = n_S. \tag{30}$$

In order to get an *a priori* approximating distribution, we determined $[S_k]/[S]$ numerically from the compact PW model and compared it with $p_k = N_k/N$, the degree distribution of the graph. Numerical results show that these are linearly related, meaning that s_k/p_k is a linear function of the degree d_k. More precisely, s_k/p_k can be written as $A(t)d_k + B(t)$, where A and B are time dependent with this relation

assumed to hold for all degrees. This allows us to deal with the heavily under determined linear system given by equations (29) and (30). Introducing the notation $q_k = s_k/p_k$, the assumption on linearity can be formulated as

$$\frac{q_k - q_1}{d_k - d_1} = \frac{q_K - q_1}{d_K - d_1}, \quad k = 1, 2, \ldots, K.$$

This yields an expression for q_k in terms of q_1, q_K and the degrees d_k as

$$(d_K - d_1)q_k = (d_k - d_1)q_K + (d_K - d_k)q_1.$$

Multiplying this equation by p_k, we get the following relation between s_k and p_k:

$$(d_K - d_1)s_k = p_k(d_k - d_1)q_K + p_k(d_K - d_k)q_1. \tag{31}$$

Observe that q_1 and q_K can be determined from system (29) and (30) by substituting the above expression for s_k. Namely, we obtain

$$(d_K - d_1) = (n_1 - d_1)q_K + (d_K - n_1)q_1, \tag{32}$$

$$(d_K - d_1)n_S = (n_2 - n_1 d_1)q_K + (n_1 d_K - n_2)q_1, \tag{33}$$

where $n_i = \sum_{k=1}^{K} d_k^i p_k$ is the ith moment of the degree distribution. (It is more convenient to use n_1 and n_2 instead of $\langle k \rangle$ and $\langle k^2 \rangle$.) Solving the linear system (32) and (33) for q_1 and q_K, we get

$$(n_2 - n_1^2)q_1 = n_2 - n_1 n_S + d_1(n_S - n_1), \tag{34}$$

$$(n_2 - n_1^2)q_K = n_2 - n_1 n_S + d_K(n_S - n_1). \tag{35}$$

Substituting these expressions into (31) leads to

$$\begin{aligned}(d_K - d_1)(n_2 - n_1^2)s_k = p_k(d_k - d_1)(n_2 - n_1 n_S + d_K(n_S - n_1))\\ + p_k(d_K - d_k)(n_2 - n_1 n_S + d_1(n_S - n_1)).\end{aligned}$$

Now we are in the position of determining the approximate second moment of the distribution s_k. Multiplying the above equation by d_k^2 and summing from $k = 1$ to $k = K$, some simple algebra yields

$$(n_2 - n_1^2)\sum_{k=1}^{K} d_k^2 s_k = n_2(n_2 - n_S n_1) + n_3(n_S - n_1).$$

Note that the third moment n_3 of the degree distribution comes into play. Thus, the desired quantity S_2 can be approximated as

$$S_2 = \sum_{k=1}^{K} d_k^2 [S_k] \approx \sum_{k=1}^{K} d_k^2 [S] s_k = [S]\frac{n_2(n_2 - n_S n_1) + n_3(n_S - n_1)}{n_2 - n_1^2}.$$

Hence, using $S_1 = [SI] + [SS] = n_S[S]$ we get

$$\frac{S_2 - S_1}{S_1^2} \approx \frac{1}{n_S^2[S]}\left(\frac{n_2(n_2 - n_S n_1) + n_3(n_S - n_1)}{n_2 - n_1^2} - n_S\right).$$

Therefore, the new closure relation is

$$[ASI] = \frac{[AS][SI]}{n_S[S]}\left(\frac{n_2(n_2 - n_S n_1) + n_3(n_S - n_1)}{n_S(n_2 - n_1^2)} - 1\right). \tag{36}$$

We note that in the case of a homogeneous network, where each node has degree n, we have $n_S = n$ and the average degree is $n_1 = n$. Hence, the expression in the bracket simplifies to $n_2/n - 1$. Moreover, the second moment is $n_2 = n^2$. Therefore, this term is simply $(n-1)$ and leads to the traditional closure $[ASI] = ((n-1)/n)([AS][SI]/[S])$.

Using the new closure (36) in the PW model (1)–(5) gives the super compact PW model in the following form:

$$[\dot{S}]_s = \gamma[I]_s - \tau[SI]_s, \tag{37}$$

$$[\dot{I}]_s = \tau[SI]_s - \gamma[I]_s, \tag{38}$$

$$[\dot{SI}]_s = \gamma([II]_s - [SI]_s) + \tau[SI]_s([SS]_s - [SI]_s)Q - \tau[SI]_s, \tag{39}$$

$$[\dot{SS}]_s = 2\gamma[SI]_s - 2\tau[SI]_s[SS]_s Q, \tag{40}$$

$$[\dot{II}]_s = -2\gamma[II]_s + 2\tau[SI]_s^2 Q + 2\tau[SI]_s, \tag{41}$$

where

$$Q = \frac{1}{n_S[S]}\left(\frac{n_2(n_2 - n_S n_1) + n_3(n_S - n_1)}{n_S(n_2 - n_1^2)} - 1\right), \quad n_S := \frac{[SI] + [SS]}{[S]}.$$

In the next section, we show that this new super compact PW model gives an as accurate output as the compact PW model, despite of the fact that it contains significantly fewer differential equations.

3. Performance of the new closure for different networks

As it was shown in Section 1 in Fig. 1, the heterogeneous PW and compact PW models give very good agreement with simulations, hence we compare the super compact PW model with the new closure to the compact PW model. This comparison will be done for different heterogeneous networks. Thus, systems (7)–(11), (16)–(20) and (37)–(41) will be solved numerically and the time dependence of $[I]_p$, $[I]_c$ and $[I]_s$ are compared, where $[I]_c = \sum_{k=1}^{N}[I_k]_c$ is the total number of infected nodes in the compact PW model. The parameters of the epidemic are fixed at $\gamma = 1$ and $\tau = 3\gamma\langle k\rangle/\langle k^2\rangle$. The later is chosen in such a way that the ratio of τ and its critical value $\tau_{cr} = \gamma\langle k\rangle/\langle k^2\rangle$ is a given constant. Here, this ratio is chosen to be 3, its actual value has only a minor influence on the results, generally this need to be greater than 1 to have an epidemic. We note that τ has been chosen to avoid the 'close to threshold' regime, where mean-field models generally fail to accurately predict simulation results [15,16].

Let us consider first the case of bimodal random graphs, where there are two different degrees d_1 and d_2, N_1 denotes the number of nodes with degree d_1 and N_2 denotes the number of nodes with degree d_2, that is, $N_1 + N_2 = N$. In order to investigate the effect of graph structure, the ratio of low and high degree nodes, i.e. N_1 and N_2, is varied. The degrees are fixed at $k_1 = 5$ and $k_2 = 35$. In Fig. 2, the curves $[I]_p$, $[I]_c$ and $[I]_s$ are shown in three cases. The average degree and the standard deviation of the degree distribution is shown in Table 1. One can see that the new system agrees with and is almost indistinguishable from the compact PW model, in fact for bimodal graphs $[I]_s$ coincides with $[I]_c$ since

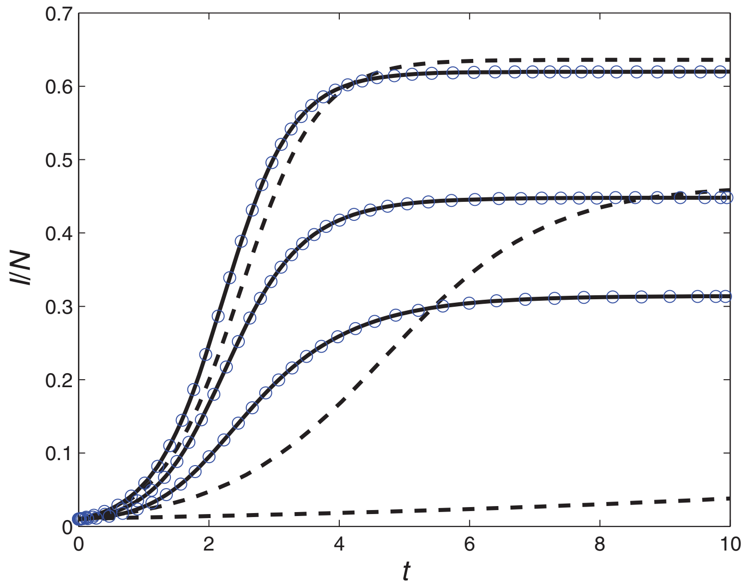

FIG. 2. The curves $[I]_p$ (dashed), $[I]_c$ (continuous) and $[I]_s$ (circles) for a bimodal graph with different ratios of the number of low and high degree nodes. The upper curves correspond to $N_1 = 0.1N$, $N_2 = 0.9N$, the middle ones are based on $N_1 = 0.5N$, $N_2 = 0.5N$ and the lower are for $N_1 = 0.9N$, $N_2 = 0.1N$. The parameter values are $N = 1000$, $k_1 = 5$, $k_2 = 35$, $\gamma = 1$ and $\tau = 3\gamma\langle k\rangle/\langle k^2\rangle$.

TABLE 1 *The average degree and the standard deviation of the degree distribution of the graphs for which the performance of the new closure was tested. For bimodal graphs the degrees are $k_1 = 5$ and $k_2 = 35$, the numbers in the first column indicate the proportion of low degree nodes, i.e. N_1/N. For the sparse power law graphs the degrees vary between $k_{\min} = 1$ and $k_{\max} = 35$, for the dense one $k_{\min} = 10$ and $k_{\max} = 140$, the power is $\alpha = 2$*

Network	$\langle k\rangle$	$\sqrt{\langle k^2\rangle - \langle k\rangle^2}$
Bimodal 0.1	32	9
Bimodal 0.5	20	15
Bimodal 0.9	8	9
Power law sparse	10.1	5.9
Power law dense	28.4	26.01

equations (29) and (30) provide a unique solution without involving any approximations. Figure 2 shows that the traditional PW model performs relatively well only in the case when the standard deviation is small, that is, the graph is nearly homogeneous.

Consider now the case of configuration random graphs with cutoff power law degree distribution. These random graphs are given by a minimal degree $k_{\min}$, a maximal degree $k_{\max}$ and a power α. The degree distribution of the graph is $p(k) = Ck^{-\alpha}$ for $k = k_{\min}, k_{\min} + 1, \ldots, k_{\max}$ with the normalization

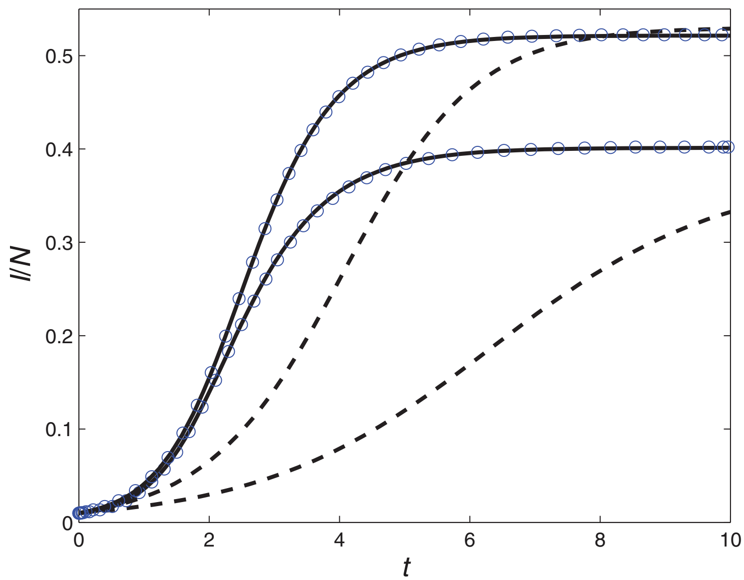

FIG. 3. The curves $[I]_p$ (dashed), $[I]_c$ (continuous) and $[I]_s$ (circles) for sparse (lower curves) and a dense (upper curves) power law configuration graphs. The lower curves belong to the sparse case with $k_{\min} = 5$ and $k_{\max} = 30$. The upper curves belong to the dense case with $k_{\min} = 10$ and $k_{\max} = 140$. The power is $\alpha = 2$ in both cases. The parameter values are $N = 1000$, $\gamma = 1$ and $\tau = 3\gamma\langle k\rangle/\langle k^2\rangle$.

constant C given by

$$\frac{1}{C} = \sum_{k=k_{\min}}^{k_{\max}} k^{-\alpha}.$$

In Fig. 3 again, the functions $[I]_p$, $[I]_c(t)$ and $[I]_s(t)$ are shown for a sparse and a dense power law configuration graph with power $\alpha = 2$. Table 1 again shows the average degree and the standard deviation of the degree distribution of the sparse and dense networks. The value of τ in both cases is $\tau = 3\gamma\langle k\rangle/\langle k^2\rangle$. We can see again that the super compact PW model gives excellent agreement with the compact PW model.

4. Epidemic threshold based on the super compact PW model

The disease-free steady state of the super compact PW models, equations (37)–(41), is given by

$$[I]_s = 0, \quad [S]_s = N, \quad [SI]_s = 0, \quad [SS]_s = n_1 N, \quad [II]_s = 0,$$
$$n_S = \frac{n_1 N}{N} = n_1 \quad \text{and} \quad Q = \frac{1}{n_1 N}\left(\frac{n_2}{n_1} - 1\right).$$

The variables of the system are $[S]_s$, $[SI]_s$, $[SS]_s$ and $[II]_s$, so the Jacobian is a 4×4 matrix. These variables are not independent because $2[SI]_s + [SS]_s + [II]_s = n_1 N$, and hence, $\lambda = 0$ will be an eigenvalue. Using the variable ordering $[S]_s$, $[SI]_s$, $[SS]_s$, $[II]_s$ and considering Q as a function of $[S]_s$, $[SI]_s$, $[SS]_s$,

i.e. $Q([S]_s, [SI]_s, [SS]_s)$, the Jacobian is

$$J = \begin{pmatrix} -\gamma & -\tau & 0 & 0 \\ A & B & +\tau[SI]_s Q & \gamma \\ C & D & E & 0 \\ F & G & H & -2\gamma \end{pmatrix},$$

where

$$A = +\tau[SI]_s([SS]_s - [SI]_s)\frac{\partial Q}{\partial [S]_s},$$

$$B = -\gamma - \tau + \tau[SS]_s Q + \tau[SI]_s[SS]_s\frac{\partial Q}{\partial [SI]_s} - 2\tau[SI]_s Q - \tau[SI]_s^2\frac{\partial Q}{\partial [SI]_s},$$

$$C = -2\tau[SI]_s[SS]_s\frac{\partial Q}{\partial [S]_s},$$

$$D = 2\gamma - 2\tau[SS]_s Q - 2\tau[SI]_s[SS]_s\frac{\partial Q}{\partial [SI]_s},$$

$$E = -2\tau[SI]_s Q - 2\tau[SI]_s[SS]_s\frac{\partial Q}{\partial [SS]_s},$$

$$F = +2\tau[SI]_s^2\frac{\partial Q}{\partial [S]_s},$$

$$G = +4\tau[SI]_s Q + 2\tau[SI]_s^2\frac{\partial Q}{\partial [SI]_s} + 2\tau,$$

$$H = +2\tau[SI]_s^2\frac{\partial Q}{\partial [SS]_s}.$$

Noting that the partial derivatives of Q are not needed because these are multiples of $[SI]_s$, which evaluates to zero at the disease-free steady state, the Jacobian at the disease-free steady state becomes

$$J\Big|_{\mathrm{DFSS}} = \begin{pmatrix} -\gamma & -\tau & 0 & 0 \\ 0 & -\gamma - \tau + \tau\dfrac{n_2 - n_1}{n_1} & 0 & \gamma \\ 0 & +2\gamma - 2\tau\dfrac{n_2 - n_1}{n_1} & 0 & 0 \\ 0 & +2\tau & 0 & -2\gamma \end{pmatrix}.$$

The characteristic polynomial is

$$(-\lambda - \gamma)\left(-\lambda - \gamma - \tau + \tau\frac{n_2 - n_1}{n_1}\right)(-\lambda)(-\lambda - 2\gamma) = 0,$$

with its eigenvalues given by

$$-\gamma, -\gamma + \tau\left(\frac{n_2}{n_1} - 2\right), 0, -\gamma.$$

The stability of the disease-free steady state changes when $\gamma = \tau(n_2/n_1 - 2)$, which is equivalent to $R_0 = 1$, with

$$R_0 = \frac{\tau}{\gamma}\left(\frac{n_2}{n_1} - 2\right) = \frac{\tau n_1}{\gamma}\left(\frac{n_2}{n_1^2} - \frac{2}{n_1}\right).$$

The best benchmark for this threshold comes form the compact PW model [7] which is

$$R_0 = \frac{\tau n_1}{\gamma}\left(\frac{n_2}{n_1^2} - \frac{1}{n_1}\right).$$

The $1/n_1$ extra term difference highlights the strong dependency of the threshold on model choice, where in this case, model coarse graining introduces a small correction/perturbation compared with the compact PW model which operates at a finer scale. Referring back to our numerical tests, we point out that we did not explicitly consider the 'close' to threshold regime, since the super compact PW model is highly coarse grained and thus unlikely to produce as good as or better agreement than more detailed or sophisticated models. This is supported by past and recent research which confirms that agreement between mean-field and simulation models close to the threshold remains difficult to obtain and often requires more sophisticated models, see [15,16].

The issue of the threshold's dependency on model and the precise value of the threshold for *SIS* dynamics on networks have recently been subject to a vigorous debate. In particular, Boguñá *et al.* [15] have recently proposed a more sophisticated mean-field model for *SIS* dynamics on networks. This model sets out to capture the global network properties and topology by considering chains of infection which go or come from much further away than the immediate neighbours that are two links away. Using this model, the authors manage to show that the epidemic threshold is vanishingly small in the thermodynamic limit in all random small-world networks with degree distribution decaying slower than exponentially.

In [16], the authors reinforce and show that different mean-field approaches lead to different outcomes in terms of the threshold. Similarly, in [17], the authors show that the heterogenous mean-field theory [3], with closures at the level of pairs, fails to correctly capture the transition point and finite-size scalings close to the threshold when a contact process dynamic is considered. They provide a heterogeneous PW-like model which produces much better agreement with simulation, and highlight again that (a) thresholds depend on the precise form of the mean-field model and (b) getting reasonable agreement between simulation and mean-field models require mean-field models at a finer scale.

5. Discussion

In this paper, we derived a super compact PW model consisting of only four equations for *SIS* dynamics and for heterogenous networks constructed according to the configuration model. This represents an improvement of going from order K, where K is the number of distinct degrees in the network, to order 1 equations, namely 4. We note that the closure that made the reduction possible relies on the observation that the distribution of susceptible nodes of degree k, which is time dependent, can be related to the original degree distribution of the network via a simple linear relation. We note that the linear relation may not be the single or unique choice, more sophisticated functional forms could be used based on combinatorial arguments. Moreover, the closure will not only encompass the first and second moment of the degree distribution but also the third. The new super compact model gives excellent agreement with the previously derived compact PW model.

The accuracy of the new closure can be estimated in a semi-analytic way. The numerical solution of the compact PW will allow us to evaluate

$$E = \frac{S_2 - S_1}{S_1^2} - Q,$$

which quantifies the performance of the newly derived closure, upon using the compact PW model as a benchmark. Moreover, it can be shown analytically that the difference $|[I]_s(t) - [I]_c(t)|$ can be estimated by a constant multiple of E.

The super compact model is a coarse grained model and it is unable to account for networks displaying preferential mixing. However, it is feasible to consider modifying the closure to account for clustering. The new model however, provides good agreement with more detailed models which are more complex to solve even numerically and offer limited analytical tractability. This model can be seen as an interpolation between full simulation and a more complex mean-field model and offers the advantage of quick insight into the impact of the network's degree distribution on epidemic dynamic. More importantly, if prevalence data are available, it is feasible to use the super compact model with a family of degree distributions or a single degree distribution with a number of parameters in order to try to infer the most likely degree distribution. This could prove to be a valuable first step before working with or developing more sophisticated models.

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