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New Moment Closures Based on A Priori Distributions with Applications to Epidemic Dynamics

Istvan Z. Kiss · Péter L. Simon

Abstract Recently, research that focuses on the rigorous understanding of the relation between simulation and/or exact models on graphs and approximate counterparts has gained lots of momentum. This includes revisiting the performance of classic pairwise models with closures at the level of pairs and/or triples as well as effective-degree-type models and those based on the probability generating function formalism. In this paper, for a fully connected graph and the simple *SIS* (susceptible-infected-susceptible) epidemic model, a novel closure is introduced. This is done via using the equations for the moments of the distribution describing the number of infecteds at all times combined with the empirical observations that this is well described/approximated by a binomial distribution with time dependent parameters. This assumption allows us to express higher order moments in terms of lower order ones and this leads to a new closure. The significant feature of the new closure is that the difference of the exact system, given by the Kolmogorov equations, from the solution of the newly defined approximate system is of order $1/N^2$. This is in contrast with the $\mathcal{O}(1/N)$ difference corresponding to the approximate system obtained via the classic triple closure. The fully connected nature of the graph also allows us to interpret pairwise equations in terms of the moments and thus treat closures and the two approximate models within the same framework. Finally, the applicability and limitations of the new methodology is discussed in detail.

Keywords Markov chain · Epidemic · Pairwise model · Closure

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1 Introduction

Graph or network theory has had a significant impact on model development and
analysis in both applied and theoretical epidemiology (Danon et al. 2011; Keeling
and Eames 2005; Newman 2003). Networks are the ideal representation of interact-
ing elements or epidemiological units, be it individuals, social groups, or even cities.
Initially, research has focused on understanding how networks evolve and grow, and
on identifying the underlying mechanisms of network processes (Newman 2003).
This has lead to a wealth of data-driven research as well as a large number of theo-
retical network models that synthesised different mechanisms of network emergence
and evolution. In parallel, the study of dynamical processes on networks evolved into
a research area in its own right. For example, individuals in a population can be rep-
resented as nodes in a network with contacts amongst individuals captured as links
amongst nodes. Assuming a simple dynamics at the node level such as the *SIS*-model
(susceptible-infected/infectious-susceptible) leads to a stochastic process where the
links in the network, and implicitly the structure of the network, will have an im-
pact on how the infection invades and spreads over the network (Danon et al. 2011;
Keeling and Eames 2005). Changing the dynamics at the node level or the struc-
ture of the network leads to different models, but from a mathematical view point all
models translate to continuous time Markov chains with extremely large state space
(M^N, where M is the number of states a node can achieve and N is the number of
nodes in the network) and given in terms of a set of Kolmogorov/master equations.
Solving these even numerically, more often than not, is challenging and impossi-
ble simply due to the large number of equations. This has led to various approaches
that set out to derive approximate models that are low-dimensional and can capture
the exact dynamics in terms of the expected values of some well-defined quanti-
ties. Early examples come from stochastically-driven spatial models from ecology
(Bolker and Pacala 1997, 1999) where moment equations are derived and their accu-
racy is investigated depending on closures at the second and third moment. Similarly,
work on lattice structured population in the context of ecology (Matsuda et al. 1992;
Sato et al. 1994) has lead to a method of constructing closed dynamical system of
overall population densities and correlation between nearest neighbours.

More recently, pairwise models (Keeling 1999) have become heavily used to cap-
ture epidemic dynamics on networks. With some similarly to earlier lattice-based
models developed in the context of ecology, this approach relies on a set of evolution
equations for the expected values of individuals of different type at the population
level (e.g., [S] and [I] the expected number of susceptible and infected nodes) which
in turn depends on the expected values of different pair types (e.g., [SI] expected
number of links connecting a susceptible to an infected node) with the hierarchi-
cal dependency on higher order structures or motifs being curtailed by a closure at
the level of triples (e.g., [SSI] expected number of triple formations with the cen-
tral S node being connected to another S and I node) in function of singles and
pairs. More rigorous approaches include the lumping technique that exploits sys-
tem symmetries and allows a significant reduction of the state space (Simon et al.
2011). Additional models such as the effective degree models (Ball and Neal 2008;
Lindquist et al. 2011) and the probability generating function (PGF) approach by

Miller (2011) and Volz (2008) led to excellent agreement with simulations without the explicit proof of convergence, but with strong probabilistic arguments based on results by Kurtz (1970) with recent results proposing a formal proof (Decreusefond et al. 2012) in the case of the *SIR* (susceptible-infected/infectious-recovered) model using the PGF or edge-based compartmental approach.

In this paper, starting from the Kolmogorov equations, given by the simple *SIS* epidemic model on a fully connected graph, the evolution equations for the moments are derived and are interpreted in terms of and compared to the classic pairwise equations. The equations for the moments are not self-contained, and a new/novel closure is proposed. This is based on the fact that the number of infecteds at all times is well approximated by a binomial distribution with time dependent parameters. The performance of the new closure is investigated numerically in the closing section and we show that this is superior to the classic closure at the level of triples used for pairwise models. In the Discussion section, we consider the applicability and limitations of our methodology and possible avenues to overcome these.

2 The New, Improved Closure Based on A Priori Distributions

2.1 Model Formulation

In this paper, we use a dynamical systems type approach, where the Kolmogorov/ master equations are simply considered as a system of linear ODEs with a transition rate matrix with specific properties such as special tri-diagonal structure and transmission rates with a well defined functional form. Consider a Markov chain with finite state space $\{0, 1, \ldots, N\}$ and denote by $p_k(t)$ the probability that the system is in state k at time t (with a given initial state that is not specified at the moment). Assuming that starting from state k, the system can move to either state $k - 1$ or to state $k + 1$, the Kolmogorov equations of the Markov chain take the form

$$\dot{p}_k = a_{k-1}p_{k-1} - (a_k + c_k)p_k + c_{k+1}p_{k+1}, \quad k = 0, \ldots, N. \tag{KE}$$

The reference model to present and test our methodology comes from epidemiology where a paradigm disease transmission model is the simple susceptible-infected-susceptible (*SIS*) model on a completely connected graph with N nodes. From the disease dynamic viewpoint, each node is either susceptible (S) or infected (I)—susceptible nodes become infected at rate τ across any link to an infectious node while infected nodes recover at rate γ and become susceptible again with all events occurring independently of each other. It is known that in this case the 2^N-dimensional system of Kolmogorov equations can be lumped to a $N + 1$-dimensional system; see Simon et al. (2011). The lumped Kolmogorov equations take again the form (KE) with

$$a_k = \tau k(N - k), \quad c_k = \gamma k \quad \text{for } k = 0, \ldots, N \text{ with } a_{-1} = c_{N+1} = 0. \tag{1}$$

2.2 Equations for the Moments

Before the main result of the paper is presented, we show how the evolution equations of the moments are derived. Let us define the jth moment associated with the stochastic process as follows:

$$y_j(t) = \sum_{k=0}^{N} \left(\frac{k}{N}\right)^j p_k(t) \quad \text{or} \quad Y_j(t) = \sum_{k=0}^{N} k^j p_k(t), \tag{2}$$

where $N^j y_j = Y_j$ with $j = 1, 2, \ldots$. The derivative of the first moment, and in a similar way all others, can be given in function of other moments upon using the Kolmogorov equations (KE). The derivation for the first moment is outlined below:

$$\dot{Y}_1(t) = \sum_{k=0}^{N} k \dot{p}_k = \sum_{k=0}^{N} k \big(a_{k-1} p_{k-1} - (a_k + c_k) p_k + c_{k+1} p_{k+1} \big)$$

$$= \sum_{k=0}^{N} (k a_{k-1} p_{k-1} - k a_k p_k - k c_k p_k + k c_{k+1} p_{k+1}).$$

By changing the indices of the summation, plugging in the corresponding expressions for the transition rates a_k and c_k (Eq. (1)) and taking into account that $a_{-1} = c_{N+1} = 0$ the following expression holds:

$$\dot{Y}_1(t) = \sum_{i=0}^{N} \big(\tau (i + i^2)(N - i) - \tau i^2 (n - i) - i^2 \gamma + (i^2 - i)\gamma \big) p_i. \tag{3}$$

Based on our notations (see, Eq. (2)), the expression above reduces to

$$\dot{Y}_1(t) = \tau N Y_1 - \tau Y_2 - \gamma Y_1 = (\beta - \gamma)Y_1 - \frac{\beta}{N} Y_2, \tag{4}$$

where $\beta = \tau N$ is the linking relation between mean-field-type and network models. Using a similar procedure, the equation for the second moment Y_2 can be easily computed and is given by

$$\dot{Y}_2 = 2(\beta - \gamma)Y_2 - 2\frac{\beta}{N} Y_3 + (\beta + \gamma)Y_1 - \frac{\beta}{N} Y_2. \tag{5}$$

Equations (4) and (5) can be recast in terms of the density dependent moments y_js to give

$$\dot{y}_1 = (\beta - \gamma)y_1 - y_2, \tag{6}$$

$$\dot{y}_2 = 2(\beta - \gamma)y_2 - 2\beta y_3 + \frac{1}{N} \big((\beta + \gamma)y_1 - \beta y_2 \big). \tag{7}$$

The derivation above relied on the convenient form (i.e., polynomial-like) of the rates but it is not restricted to simple epidemic dynamics on fully connected graphs. While

the above equations are exact, the system is not self-contained since the second moment depends on the third and an equation for this is also needed. It is easy to see that this hierarchical dependence of moments leads to an infinite but countable number of equations; see Bátkai et al. (2012), Simon and Kiss (2011). Hence, to derive a tractable system at the level of moments, a *closure* is needed. The same line of thinking applies to many mean-field type approximate models such as the pairwise model where the expected number of singles (e.g., susceptible and infecteds) depends on doubles/pairs which in turn depend on triples with this chain being closed by approximating triples in term of singles and pairs; see Keeling (1999). Below, we give the main result of the paper in the form of a new closure based on an a priori assumption about the distribution of the infecteds.

2.3 Derivation of the New Closure

The novel closure put forward here is based on the empirical observation that $p_k(t)$ is well approximated by a binomial distribution $\mathcal{B}(n, p)$, where n and p depend on time and will be given in terms of the moments of the distribution. The first three moments of the binomial distribution can be specified easily in terms of the two parameters and are as follows:

$$Y_1 = np, \tag{8}$$

$$Y_2 = np + n(n-1)p^2, \tag{9}$$

$$Y_3 = np + 3n(n-1)p^2 + n(n-1)(n-2)p^3. \tag{10}$$

Using Eqs. (8) and (9), n and p can be expressed in term of Y_1 and Y_2 as follows:

$$p = 1 + Y_1 - \frac{Y_2}{Y_1}, \qquad n = \frac{Y_1^2}{Y_1 + Y_1^2 - Y_2}. \tag{11}$$

Plugging the expressions for p and n (Eq. (11)) into Eq. (10), the closure for the third moment is found to be

$$Y_3 = \frac{2Y_2^2}{Y_1} - Y_2 - Y_1(Y_2 - Y_1). \tag{12}$$

This relation defines the new triple closure and in terms of the density dependent moments is equivalent to

$$y_3 = \frac{2y_2^2}{y_1} - y_1 y_2 + \frac{1}{N}(y_1^2 - y_2). \tag{13}$$

Using the equations for the first moment (6) the closure at the level of the pairs yields the following approximate equation

$$\dot{x}_1 = (\beta - \gamma)x_1 - \beta x_1^2. \tag{14}$$

Using the equations for the first two moments ((6) and (7)) and the closure at the level of the third moment yields

$$\dot{x}_1 = (\beta - \gamma)x_1 - \beta x_2, \tag{15}$$

$$\dot{x}_2 = 2(\beta - \gamma)x_2 - 2\beta x_3 + \frac{1}{N}\big((\beta + \gamma)x_1 - \beta x_2\big), \tag{16}$$

where

$$x_3 = \frac{2x_2^2}{x_1} - x_1 x_2 + \frac{1}{N}\big(x_1^2 - x_2\big). \tag{17}$$

Moreover, we can also define a simplified binomial closure by neglecting the order $1/N^2$ in the full binomial closure, provided also that $x_1^2 - x_2$ is of $\mathcal{O}(1/N)$. This will lead to

$$x_3 = 3x_1 x_2 - 2x_1^3. \tag{18}$$

It is worth to note that the above closure (Eq. (18)) follows from the same calculation upon assuming that the a priori distribution is *Normal* rather than *Binomial*. To carry out the same calculation Eqs. (8)–(10) need to be modified to reflect the moments of the *Normal* distribution.

The use of a fully connected graph opens up many avenues to compare and relate the newly derived closure to existing ones. In particular, we harness the power of this opportunity by exploring, both rigorously and numerically, how the new closure performs relative to the well-established, classic triple closure. Furthermore, the fully connected graph allows us to make comparisons directly to the exact system which is computable.

3 Pairwise Models: Closure Relations and Their Performance

It is of great interest to understand how and when the full set of Kolmogorov equations can be approximated via low-dimensional ODEs and also to assess the performance of the approximate models by, for example, working out the rate of convergence of the exact/full model towards the solution of the approximate or mean-field model or simply estimating the absolute difference between the two. Pairwise models have been widely used as an alternative or as a companion to simulation of epidemic models on mainly homogeneous random graphs. While originally, the pairwise equations have not been directly linked to the exact Kolmogorov equations, more recently, Simon et al. (2011) and Taylor et al. (2011) have shown that these can be derived directly from the exact Kolmogorov equations and that the pairwise equations are also exact on any arbitrary network before a closure is applied. Focusing on the simple *SIS* type model, the first moment of the distribution is given by

$$[\dot{I}] = \tau[SI] - \gamma[I], \tag{19}$$

where $[I](t) = \sum_{k=0}^{N} k p_k(t)$. This is not a closed equation since $[SI]$ itself is a variable and an equation for this is needed. However, we can look for an approximation

whereby the expected number of edges $[SI] \simeq e_{[SI]}([I]) = [I](N - [I])$, that is, the expected number of (SI) pairs is estimated in terms of the number of the expected number of infecteds $[I]$. This now leads to a self-contained equation in terms of a new approximate variable $\tilde{I}$ given by

$$\dot{\tilde{I}} = \tau \tilde{I}(N - \tilde{I}) - \gamma \tilde{I}. \tag{20}$$

This is the well-known compartmental model for the *SIS* epidemic.

The same argument can repeated by using a closure at the level of triples rather then pairs. In this case, the exact pairwise equations are given by

$$\frac{d[I]}{dt} = \tau[SI] - \gamma[I], \tag{21}$$

$$\frac{d[SI]}{dt} = \gamma([II] - [SI]) + \tau([SSI] - [ISI] - [SI]), \tag{22}$$

$$\frac{d[II]}{dt} = -2\gamma[II] + 2\tau([ISI] + [SI]), \tag{23}$$

$$\frac{d[SS]}{dt} = 2\gamma[SI] - 2\tau[SSI]. \tag{24}$$

Using the well-known closure given by $[ABC] = \frac{N-2}{N-1} \frac{[AB][BC]}{[B]}$ (see House and Keeling 2010, 2011; Keeling 1999) leads to the following approximate system:

$$\dot{\overline{I}} = \tau \overline{SI} - \gamma \overline{I}, \tag{25}$$

$$\dot{\overline{SI}} = \gamma(\overline{II} - \overline{SI}) + \tau(\overline{SSI} - \overline{ISI} - \overline{SI}), \tag{26}$$

$$\dot{\overline{II}} = -2\gamma \overline{II} + 2\tau(\overline{ISI} + \overline{SI}), \tag{27}$$

$$\dot{\overline{SS}} = 2\gamma \overline{SI} - 2\tau \overline{SSI}. \tag{28}$$

The focus now shifts from the derivation of the approximate model to whether and how well these agree with output from the exact system. More precisely, we will simply consider the difference between the exact solution $[I]$ and the approximate solutions $\tilde{I}$ and $\overline{I}$ in terms of the magnitude of $\|[I](t) - \tilde{I}(t)\|$ and $\|[I](t) - \overline{I}(t)\|$, and how these depend on population or network size. Numerical investigation reveals that the difference is of order $1/N$ for closures both at the level of pairs and triple. This is shown in Fig. 1, where both the exact (Eq. (KE) with coefficients given by Eq. (1)) and the approximate systems (i.e., with pairwise closure given by Eq. (20) and triple closure given by Eqs. (25)–(28)) have been solved numerically. This is somewhat surprising given that, at least intuitively, it is expected that the closure at the level of triples will be superior to that at the level of pairs. This numerical result can be made more rigorous at least for the closure at the level of pairs as shown by Bátkai et al. (2012) and Simon and Kiss (2011).
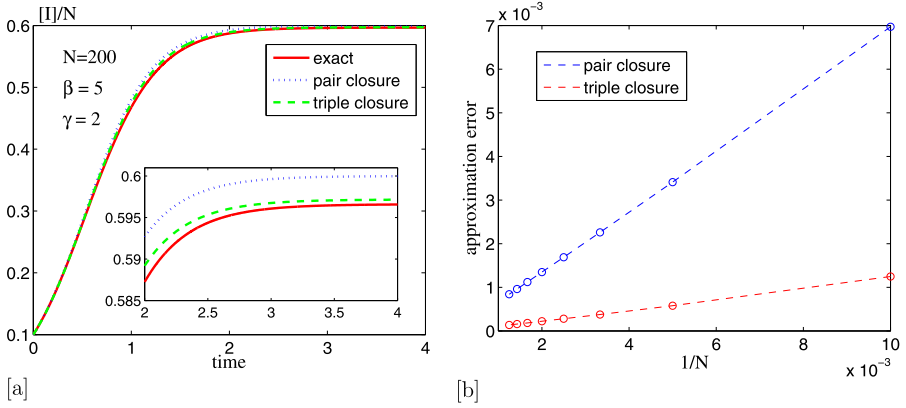
Fig. 1 (**a**) Time evolution of the fraction infected (prevalence) based on the exact model and two different closures; pair and triple level. Here, $N = 200$, $\gamma = 2$, and $\beta = 5$. (**b**) Approximation error (absolute value of the difference between the exact and two approximate models at steady state) plotted for different system sizes for the same transmission and recovery parameter values as at (**a**)

4 Interpreting Pairwise Equations and Closures in Terms of Moments

4.1 The Equivalence Between Pairwise and Moment Equations

To be able to link the pairwise approach to the moment approach, it is necessary to count the expected value of the singles, pairs, and triples in terms of the moments. For a fully connected graph, this is straightforward. For example, based on Eq. (2), the expected number of infecteds is given by

$$[I](t) = \sum_{k=0}^{N} k p_k(t) = N y_1(t). \tag{29}$$

Following the same approach, it is easy to show that similar identities for pairs and triples can be derived. For example,

$$[SI](t) = \sum_{k=0}^{N} k(N-k) p_k(t) = N^2 \sum_{k=0}^{N} \frac{k}{N} \left(1 - \frac{k}{N}\right) p_k(t) = N^2 \big(y_1(t) - y_2(t)\big), \tag{30}$$

where, $k(N-k)$ simply denotes the number of (SI) pairs on a fully connected graph with N nodes and k infected individuals. For triples, the calculations are equally intuitive. For example, the expected number of $[SSI]$ triples can be counted by averaging over $(N-k)(N-k-1)k$—the number of $[SSI]$ triples in the presence of k infected nodes. Hence, the following relation holds:

$$[SSI](t) = \sum_{k=0}^{N} (N-k)(N-k-1)k p_k(t)$$

$$= N^3 \sum_{k=0}^{N} \left(1 - \frac{k}{N}\right)\left(1 - \frac{k}{N} - \frac{1}{N}\right)\frac{k}{N} p_k(t)$$

$$= N^3 \left(\left(1 - \frac{1}{N}\right)y_1(t) + \left(\frac{1}{N} - 2\right)y_2(t) + y_3(t)\right). \tag{31}$$

Following the same simple procedure as above, the following relations hold:

$$[S](t) = N(1 - y_1(t)), \tag{32}$$

$$[II](t) = N^2\left(y_2(t) - \frac{1}{N}y_1(t)\right), \tag{33}$$

$$[SS](t) = N^2\left(1 - \frac{1}{N} + \left(\frac{1}{N} - 2\right)y_1(t) + y_2(t)\right), \tag{34}$$

$$[ISI](t) = N^3\left(-\frac{1}{N}y_1(t) + \left(\frac{1}{N} + 1\right)y_2(t) - y_3(t)\right). \tag{35}$$

The results above allows us to test if the equations for the moments are consistent with the pairwise ones. Starting from the equation for the expected number of infecteds and upon using Eq. (6), we obtain

$$[\dot{I}](t) = N\dot{y}_1(t) = N\big((\beta - \gamma)y_1 - y_2\big) = N\big(\beta(y_1 - y_2) - \gamma y_1\big) = \frac{\beta}{N}[SI] - \gamma[I]. \tag{36}$$

The calculations above can be repeated for all other equations and these confirm the one-to-one correspondence between the moment and pairwise equations.

4.2 Interpreting Closures via Moments

The closure at the level of pairs and triples have to equally translate in a relation between the moments. First, the closure at the level of pairs is discussed. We look to use the pairwise closure $[SI] = [S][I] = (N - [I])[I]$ to obtain a relation between the moments. The simple relation above in terms of the moments translates to

$$N^2\big(y_1(t) - y_2(t)\big) = N^2\big(y_1(t) - y_1^2(t)\big) \quad \Leftrightarrow \quad y_2(t) = y_1^2(t). \tag{37}$$

For the triple closure, the situation is different in that two different triples are closed, albeit using the same formal relation, and this could potentially lead to two different relations between the moments. The first triple closure, for the SSI triple, upon using Eqs. (30)–(32) and (34), leads to the following relation:

$$\left(1 - \frac{1}{N}\right)y_1 + \left(\frac{1}{N} - 2\right)y_2 + y_3 = \frac{N-2}{N-1}\frac{(1 - \frac{1}{N} + (\frac{1}{N} - 2)y_1 + y_2)(y_1 - y_2)}{1 - y_1}. \tag{38}$$

The equation above, after some algebra, yields a closure at the level of the moments and y_3 can be given in function of the previous two moments as follows:

$$y_3 = -\frac{1}{N}y_1 + \left(1 + \frac{1}{N}\right)y_2 - \frac{N-2}{N-1}\frac{(y_1 - y_2)^2}{1 - y_1}. \tag{39}$$

It is worth noting that the closure for [*ISI*] yields the same closure relation for the third moment.

To summarise, we make the following observations:

1. The closed system for the moments reduce to two simple ODEs and this is in contrast with four equations for the pairwise model. However, this apparent discrepancy is not as marked since the pairwise model can be easily reduced to three equations by noting that, for example, $[SS] = (N − 1)(N − [I]) − [SI]$. This still leaves one extra equation in the pairwise model when compared to the equivalent system in terms of moments. This suggests that the three equations are not completely independent in some sense that is not easy to define or pinpoint.
2. The use of fully connected graphs allowed us to count pairs and triples in a straight forward way and to identify the one-to-one correspondence between pairwise and moment equations. This does not preclude the applicability of our methodology to other scenarios, but it may mean that linking the newly derived approximate model to other existing ones may not be obvious or even impossible. However, as long as the approximation is valid and performs well, comparisons to other models can still be made via numerical methods.

5 The Performance of Triple and Newly-Derived Closure on a Fully Connected Graph

The current setup allows us to compare the exact model as given by the Kolmogorov equations (KE) with transition rates given by Eq. (1) to three different approximate models. The first results from the pairwise closure and is given by Eq. (20). The second is a direct consequence of the closure at the level of triples and is given by Eqs. (25)–(28). Finally, the third approximate system results from the novel binomial closure (see Eq. (13)) with the approximate system defined by Eqs. (15)–(17). The elegance of this approach stems from the fact that all numerical results are free from simulations and rely solely on the time integration of ODE systems. In Fig. 1, plots of the time evolution together with the approximation errors are given for the classic approximate models corresponding to pairwise and triple closure. The most significant feature of this plot is the order $1/N$ approximation error independently of the closure. The same approximation error suggests qualitative similarity between the two approximate models and it somewhat surprising that the closure at the level of triples produces no immediately obvious benefits or qualitatively different behaviour. In contrast, in Fig. 2, the performance of the binomial closure is compared to the triple closure. The approximation error plot in Fig. 2b is the most significant as it shows numerical evidence that the binomial closure performs significantly better with error that is of order $1/N^2$. While we were not yet able to prove analytically this result, for the case of pairwise closure we gave rigorous proof in Bátkai et al. (2012) and Simon and Kiss (2011), where the result is more general as apart from estimating the approximate error at the steady state also extends to the approximate error at different times.

The quantitative comparison of the different closure relations is shown in Table 1. Here, the values of the steady states obtained for the different closures are compared
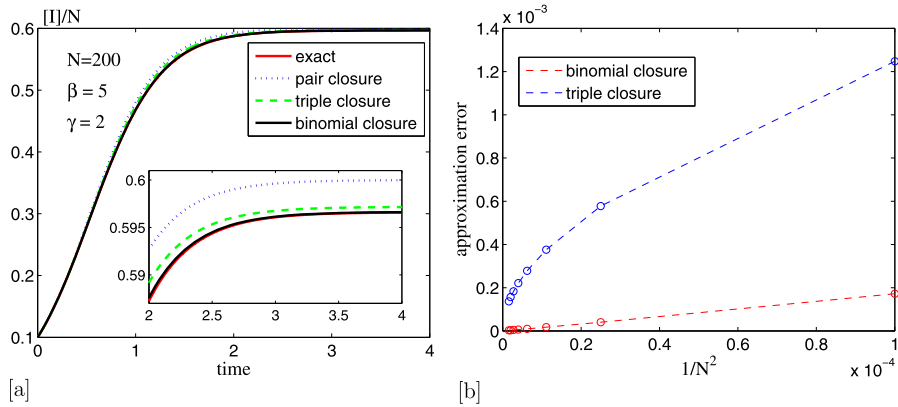
Fig. 2 (**a**) Time evolution of the fraction infected (prevalence) based on the exact model and three different closures; pair, triple level, and the binomial closure. Here, $N = 200$, $\gamma = 2$ and $\beta = 5$. (**b**) Approximation error (absolute value of the difference between the exact and approximate models at steady state given by the triple and binomial closures) plotted for different system sizes for the same transmission and recovery parameter values as at (**a**). It is worth noting that the x-axis in (**b**) is in terms of $1/N^2$ as opposed to $1/N$ as in Fig. 1b

Table 1 Numerical values for the discrepancy between the exact and approximate solutions at the steady state for different network sizes

N	100	200	400	800
$1000 \times$ pair appr. err.	6.9486	3.4008	1.6832	0.8374
$1000 \times$ triple appr. err.	1.2355	0.5729	0.2763	0.1357
$1000 \times$ binomial appr. err.	0.1689	0.0395	0.0096	0.0024

to the exact value of the stationary prevalence. The advantage of comparing the steady state values is that these can be given analytically without solving ODEs numerically. The steady state from the pairwise closure Eq. (20) is

$$\frac{\tilde{I}_{ss}}{N} = 1 - \frac{\gamma}{\beta}, \tag{40}$$

where $\beta = \tau N$. The steady state from the triple closure Eqs. (25)–(28) is

$$\frac{\overline{I}_{ss}}{N} = (N-1)\frac{(N-2)\beta - N\gamma}{(N-1)(N-2)\beta - N\gamma}. \tag{41}$$

The steady state from the binomial closure Eqs. (15)–(17) is

$$\frac{I_{ss}^*}{N} = \frac{Nq^2 - 1}{Nq - 1}, \tag{42}$$

where $q = 1 - \gamma/\beta$. Finally, the value of the steady state from the Kolmogorov equations (KE) can be derived as

$$\frac{[I]_{ss}}{N} = \frac{\sum_{k=0}^{N-1}(k+1)A_k}{N\sum_{k=0}^{N-1}A_k}, \tag{43}$$

where $A_0 = 1$ and

$$A_k = \frac{\beta^k(N-1)(N-2)\cdots(N-k)}{\gamma^k(k+1)N^k}, \quad k = 1, 2, \ldots, N-1.$$

The approximation errors shown in Table 1 are

$$\left|\frac{\tilde{I}_{ss}}{N} - \frac{[I]_{ss}}{N}\right|, \quad \left|\frac{\overline{I}_{ss}}{N} - \frac{[I]_{ss}}{N}\right|, \quad \left|\frac{I_{ss}^*}{N} - \frac{[I]_{ss}}{N}\right|.$$

In the table, these values are multiplied by 1000 to get numerical values closer to 1. Using the analytical expressions above, it is easy to show that $\frac{\overline{I}_{ss}}{N} \to \frac{\tilde{I}_{ss}}{N}$ and $\frac{I_{ss}^*}{N} \to \frac{\tilde{I}_{ss}}{N}$ when $N \to \infty$. However, we did not yet manage to formally prove that

$$\left|\frac{\tilde{I}_{ss}}{N} - \frac{[I]_{ss}}{N}\right|/N, \quad \left|\frac{\overline{I}_{ss}}{N} - \frac{[I]_{ss}}{N}\right|/N, \quad \left|\frac{I_{ss}^*}{N} - \frac{[I]_{ss}}{N}\right|/N^2$$

all tend to a nonzero number as N gets large, and thus analytically confirming the $\mathcal{O}(1/N)$ and $\mathcal{O}(1/N^2)$ errors.

6 Discussion

In this paper, we proposed a novel closure that produces qualitatively different results when compared to the classic closure. Namely, the difference between the exact system from the solution of the approximate model that results from the binomial closure is smaller (i.e., $\mathcal{O}(1/N^2)$ compared to $\mathcal{O}(1/N)$) and this has been illustrated via numerical examples. The use of a fully connected graph allowed us to identify an exact correspondence between the equations of the moments and pairwise equations as well as the two different closure relations. This has meant that two different models could be analyzed within the same framework and results from the approximate models could be compared directly to the numerical solution of the exact system.

The procedure that we illustrate in this paper can be generalized and applied within the context of model reduction, where Kolmogorov-type systems are reduced to approximate models with far fewer equations. Our method is based on a semiheuristic argument which relies on the assumption that the distribution of the stochastic process in time can be well-approximated by some theoretical distribution with time-dependent parameters. Moreover, the distribution has to be such that there is a unique, one-to-one correspondence between the moments and the parameters of the distribution. If the conditions above hold, the theoretical distribution will determine the exact type of closure that is necessary to obtain a reduction in the number of equations.

The method also allows us to close at different moments and to explore the benefits of closing at lower or higher order moments. For example, one can attempt to close the moment equations at the second moment but, without using the equivalent closure that follows from the pairwise model. This can be achieved by considering the limiting case of $n = N$ and expressing the second moment in terms of the first. This will lead to a new closure at the level of pairs, but this performs similarly to the classic closure at the pair level.

While the initial results and applicability of our method is promising (see example below for the Erdős–Rényi random graph case), we are yet to fully explore the applicability of our method or to identify the sufficient and/or necessary requirements that guarantees that the proposed closure or reduction procedure will be applicable. It is worth noting that here the main focus in not on the approximation of simulation results corresponding to a stochastic process but rather the model reduction where the Kolmogorov equations are already given and accepted as a valid model.

A natural extension of our methodology would be to consider the same epidemic dynamics on Erdős–Rényi random graphs, where the average degree of nodes is denoted by $n(\ll N)$. Despite the resulting exact model requiring a state space that is much larger than N (i.e., with 2^N elements), we propose to work with an approximate version over a state space of size $N + 1$ and with the transition rates given by

$$a_k = \tau n k \frac{N - k}{N - 1}, \quad c_k = \gamma k \quad \text{for } k = 0, \dots, N \text{ with } a_{-1} = c_{N+1} = 0. \quad (44)$$

The above approximate model ignores the natural correlations that will develop and operates on the assumption of random mixing. This means that although the natural disease transmission process will lead to different arrangements of k infectious individuals on the network, and thus different counts for the various pair types, the model above takes an average over all configurations and assumes that Ss and Is are randomly distributed on the network. However, with the applicability of our methodology in mind, we note that the above model has the potential to be refined in order to provide an improved approximation of the true, exact model. This can be achieved by deriving the transmission rates a_k ($k = 0, 1, \dots, N$), be it based on some combinatorial or random walk argument, in a way in which a_k will take into account at least some of the natural correlations. To support our statement, in Fig. 3, we plot the time evolution of the expected prevalence from simulation and from Kolmogorov equations with a_k taken as an average from simulation, namely $a_k = \tau e_{[SI]}(k)$, where $e_{[SI]}(k)$ is the expected number of (SI) pairs in the presence of k infected nodes on the network. The excellent agreement shows that it is feasible to attempt to derive transmission rates based on some analytic or semianalytic approaches. Depending on the intended use of our methodology, the issue of the exactness of the Kolmogorv equations may or may not be an issue. For example, if one accepts the Kolmogorov equations as a given and valid model, our methodology can be perceived as a method of approximating Kolmogorov equations via low-dimensional ODEs in terms of the moments.

While there are limitations to the extension of our results to arbitrary graphs and/or dynamics, the present paper provides the basis for some more rigorous analysis as
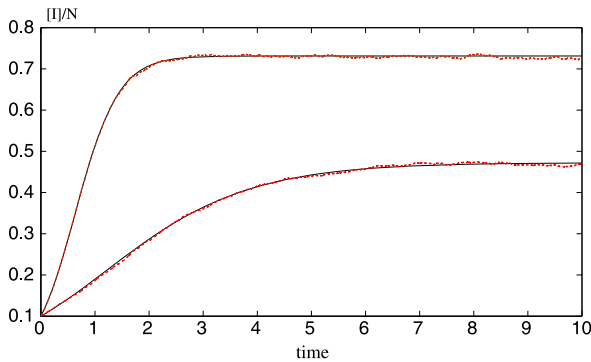
Fig. 3 Time evolution of the fraction infected (prevalence) based on simulation (*dashed lines*) and the approximate Kolmogorov equations (*continuous lines*) with transmission rates a_k with ($k = 0, 1, \ldots, N$) taken as expected values from the simulation. Here, the networks are Erdős–Rényi random with $N = 100$, and average degree $n = 10$, with $\gamma = 1$, $\tau = 0.2$ (*lower*) and $\tau = 0.4$ (*upper*). All simulations start with 10 infected nodes chosen at random and the average is based on 250 individual realizations

well as the possibility of deriving new closures. As such, this study offers a new or different direction that can lead to further progress in the area of approximating stochastic processes independently of whether these involve networks.

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