Solvability of implicit final size equations for SIR epidemic models

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Abstract

Final epidemic size relations play a central role in mathematical epidemiology. These can be written in the form of an implicit equation which is not analytically solvable in most of the cases. While final size relations were derived for several complex models, including multiple infective stages and models in which the durations of stages are arbitrarily distributed, the solvability of those implicit equations have been less studied. In this paper the SIR homogeneous mean-field and pairwise models and the heterogeneous mean-field model are studied. It is proved that the implicit equation for the final epidemic size has a unique solution, and that through writing the implicit equation as a fixed point equation in a suitable form, the iteration of the fixed point equation converges to the unique solution. The Markovian SIR epidemic model on finite networks is also studied by using the generation-based approach. Explicit analytic formulas are derived for the final size distribution for line and star graphs of arbitrary size. Iterative formulas for the final size distribution enable us to study the accuracy of mean-field approximations for the complete graph.

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1   Introduction

Deriving final epidemic size relations is a central question in mathematical epidemiology. The final size of an epidemic can be defined informally as the total number of individuals experiencing infection during the outbreak. This quantity yields the attack rate expressed as a percentage of the population in question. The final size of an epidemic can be defined for SIR-type epidemic processes, when individuals are initially susceptible then become infected due to interactions with infected individuals, and eventually, infected individuals recover, and do not affect the process further. Assuming a deterministic model, we use $S(t)$, $I(t)$, and $R(t)$ to denote the number of susceptible, infected, and recovered individuals at time t in a population of fixed size N, that is $S(t) + I(t) + R(t) = N$. The aim is to determine $R(\infty)$, the large time limit of the size of the recovered class, called the final epidemic size. Note that this includes the number of initially infected individuals. For stochastic models, the final size distribution, p_k, is the main target of the investigation, defined as the probability of having k recovered individuals when the process is finished, i.e. when there are no more infected individuals. The final epidemic size can be then defined as the expected value of this distribution: $R_\infty = \sum k p_k$. We note that considering the possible bimodality of the distribution, the final size is sometimes defined as the conditional expected value given that there is a large outbreak. (The bimodal nature of the distribution close to the threshold is studied in more detail in Section 5.2.)

Final epidemic size relations have been widely studied starting from the simplest SIR compartmental model via network epidemic models to mean-field approximations. In early works, the case of homogeneous mixing was considered, see e.g. [4, 14, 22], and the final epidemic distribution was derived for different epidemic processes. It is emphasised in [20] that the final size results obtained for the Reed–Frost model can be extended to a wide range of other models. The final size distribution for that model is described in [21]. The homogeneous mixing assumption was released in a series of papers by Ball and coworkers for populations with two levels of mixing, see e.g. [7, 8]. In order to increase heterogeneity, the household structure of the population is also taken into account in [6], and global contacts are made through the edges of a random graph with a given degree distribution in [9], where household structure is also considered.

In [15] a final size relation is derived for models with multiple infective stages and models in which the durations of stages are arbitrarily distributed, while keeping the homogeneous mixing assumption. In [3] a final size relation is derived for models in which there are multiple susceptible classes, such as models including vaccination. Moreover, the final size formula is related to the basic reproduction number. This relation is extended to more general models including a subdivided population with general mixing patterns among subgroups [2]. In that paper it is proved that the final size equation determines a unique value for the final epidemic size. The stochastic models can be studied by the branching process approach, see e.g. [8], where the final size distribution is determined for contact structures under very weak constraints on the prescribed degree distribution. These results are asymptotic, in that they require the total population size tend to infinity for them to be exact. The stochastic model with heterogeneous infectivity and susceptibility has also been studied in [17]. A large number of approaches to calculate the final-size distribution are reviewed in [12] with paying particular attention to numerical implementation, including a novel application for iterative methods. The iterative method is used in [11] to develop a new methodology for the efficient computation of epidemic final size distributions for a broad class of Markovian models, applied in particular to SIR epidemic

on complete graphs. An alternate approach to deriving final sizes is suggested in [18]. This approach directly considers the underlying stochastic process of the epidemic rather than the approximating deterministic equations and gives insight into why the relations hold. Closed-form analytic expressions for the mean and variance of the number of infectious individuals as a function of time and the degree of the initially infected individuals is shown in [5].

The final size of an SIR epidemic was studied also for mean-field network models. The final size relation for the pairwise model (closed at the level of triples) was derived in [13], and for the heterogeneous mean-field model (closed at the level of pairs) in [19]. In [16] analytical expressions for the final epidemic size of an SIR model are derived for small networks composed of three or four nodes with different topological structure.

While final size relations were derived for several complex models, the solvability of those implicit equations have been less studied. In this paper we study three mean-field models, namely the homogeneous mean-field and pairwise models and the heterogeneous mean-field model. For these models we prove that the implicit equation for the final epidemic size has a unique solution for an arbitrary set of the model parameters. Moreover, we show that, writing the implicit equation as a fixed point equation in a suitable form, the iteration of the fixed point equation converges to the unique solution. Besides these mean-field approximations, we also study the Markovian stochastic SIR model of epidemic propagation on finite networks that will be referred to as exact stochastic model. This model can be studied by using the generation-based approach. This approach can be carried out for graphs with special structure. Here we derive explicit analytic formulas for the final size distribution for line and star graphs of arbitrary size. The iterative method developed in [11] is used to determine the final size distribution for the complete graph, enabling us to study the accuracy of mean-field approximations.

The paper is structured as follows. The final size implicit equations are derived and their solvability is proved for the homogeneous mean-field approximation in Section 2, for the homogeneous pairwise model in Section 3 and for the heterogeneous mean-field model in Section 4. The mean-field approximations are compared to the exact stochastic model for a complete graph in Section 5. The exact analytic formulas for the final size distribution are derived in Section 5.1 for the line and star graphs by using a recursive method. The paper concludes with a discussion section.

2 Homogeneous mean-field model

As a simplest mean-field approximation we consider first the following system of ordinary differential equations, which is the homogeneous mean-field approximation of SIR epidemic dynamics in a homogeneous network, where each node is assumed to have the same degree [13].

$$[\dot{S}]_f = -\tau \frac{n}{N} [S]_f [I]_f, \tag{1}$$

$$[\dot{I}]_f = -\gamma [I]_f + \tau \frac{n}{N} [S]_f [I]_f, \tag{2}$$

$$[\dot{R}]_f = \gamma [I]_f, \tag{3}$$

where $[S]_f(t)$, $[I]_f(t)$, $[R]_f(t)$ denote the mean-field approximation of the expected value of the number of susceptible, infected and recovered nodes at time t, respectively, the subscript "f" refers to "first" since this can be considered as the first approximation when

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the number of pairs is expressed in terms of the number of singles. The parameters τ and γ are the per-contact infection rate and the recovery rate, n is the average degree of the network. It can be easily seen that the three differential equations are not independent since the conservation equation $[S]_f(t) + [I]_f(t) + [R]_f(t) = N$ holds, where N denotes the total number of nodes in the network. We note that this system is obtained from the exact system by using the pair closure approximation $[SI] \approx \frac{n}{N}[S][I]$. The main characteristic of this model is the final epidemic size $R_\infty = \lim_{t \to \infty} [R]_f(t)$. We note that the proper notation would be R_∞^f, since this quantity is given by the first approximation and hence differs from the exact value of the final epidemic size. However, for the sake of simplicity we omit the superscript "f". The final epidemic size can be obtained from an implicit equation that can be derived from the differential equations, see e.g. [18, 19], and also from the stochastic formulation of the model, see for example Section 4.3 of [1]. Our goal with exploring this model is to prove the existence and uniqueness of the solution of this implicit equation and to show that simple iteration converges to the unique solution. For the Reader's convenience we also show a simple derivation of the implicit equation following [18].

2.1   Derivation of the implicit equation for the final epidemic size

when there are no more infected individuals, the epidemic reaches completion, so we have $S_\infty + R_\infty = N$. For simplicity we assume $[R]_f(0) = 0$, so $[S]_f(0) + [I]_f(0) = N$. We can rewrite equation (1) as $[\dot{S}]_f + \tau \frac{n}{N}[S]_f[I]_f = 0$. Based on (3) this can be written as $[\dot{S}]_f + \frac{\tau n}{\gamma N}[S]_f[\dot{R}]_f = 0$. Using the integrating factor $\exp(\frac{\tau n}{\gamma N}[R]_f)$ we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\left(e^{\frac{\tau n}{\gamma N}[R]_f(t)}[S]_f(t)\right) = 0.$$

Integrating this and using $[R]_f(0) = 0$ leads to $[S]_f(t) = S_0 e^{-\frac{\tau n}{N\gamma}[R]_f(t)}$, where $S_0 = [S]_f(0)$. Taking the limit $t \to \infty$ and using $S_\infty + R_\infty = N$, we conclude

$$R_\infty = N - S_0 e^{-\frac{\tau n}{\gamma N}R_\infty}. \tag{4}$$

2.2   Existence and uniqueness of the solution of the implicit equation

Now our aim is to prove that (4) has a unique positive solution R_∞ for any $S_0 \in [0, N)$. We note that dividing (4) by N (in the case $S_0 = N$) yields a fixed point problem which is equivalent to that arising when the extinction probability of a Galton-Watson process with a Poisson offspring distribution is considered. The existence result for the case $S_0 = N$ then follows from standard branching process theory. However, for the Reader's convenience and in order to make the paper self-contained, we present the simple proofs below. In the case when there are no infected nodes initially, i.e. $S_0 = N$, all nodes remain susceptible, that is we have the trivial solution $R_\infty = 0$. We note that it is interesting to investigate the limit of R_∞ as S_0/N tends to 1. If this limit is zero then we do not have an epidemic with a small initial infection (i.e. with I_0/N tending to zero.) However, it may happen that the limit is positive, meaning that even a very small initial infection can lead to a positive final epidemic size. Our derivation will yield the threshold value of the infection rate τ separating these two behaviours.

Introducing the notation $B = \tau n/\gamma N > 0$, the solution of (4) can be obtained as the fixed point of the function $f(x) = N - S_0 e^{-Bx}$, that is $R_\infty = x^*$, where x^* satisfies

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$f(x^*) = x^*$. This observation enables us to reduce the question of solvability of equation (4) to finding the fixed point of a function, leading to the following proposition.

Proposition 1 *If $S_0 \in [0, N)$, then (4) has a unique positive solution R_∞. If $S_0 = N$, then (4) has a trivial solution $R_\infty = 0$. Moreover, if $S_0 = N$ and $\tau n > \gamma$, then (4) has a positive solution besides the trivial solution.*

PROOF: The existence of the solution in the case $S_0 < N$ follows directly from the continuity of f and the facts that $f(0) = N - S_0 > 0$ and $f(N) = N - S_0 e^{-BN} < N$. Namely, the inequalities imply that the graph of the function starts above the diagonal $y = x$ and ends below that line segment, hence it has an intersection with the diagonal. For the uniqueness it is enough to show that the graph has a unique intersection point with the diagonal. This follows easily from the fact that the graph is concave that can be seen from the fact that the second derivative of f is negative in the interval $[0, N]$, $f''(x) = -S_0 B^2 e^{-Bx} < 0$. Let us turn to the case $S_0 = N$. In this case $f(0) = 0$, hence we have the trivial fixed point $x^* = 0$. Since the graph of f is concave, it is the only solution if the graph starts below the diagonal, that is $f'(0) < 1$. However, in the case $f'(0) > 1$, the graph starts above the diagonal and ends below it, hence there is a further solution in the positive region. Since $f'(x) = S_0 B e^{-Bx}$ and $S_0 = N$, the condition $f'(0) > 1$ is equivalent to $\tau n > \gamma$, yielding the desired statement.
□

2.3   Solving the implicit equation numerically by iteration

Now we show how the solution of (4) can be found by using an iteration. Since the equation is in the form of a fixed point equation the natural iteration is $x_{n+1} = f(x_n)$. First we give a sufficient condition on f ensuring that this iteration converges to the unique fixed point of f.

Lemma 1 *Let $f : I \to I$ be a strictly increasing continuous function on the interval I that has a unique fixed point $x^* \in I$ satisfying $f(x^*) = x^*$. Moreover, assume that $f(x) > x$ holds for $x < x^*$ and $f(x) < x$ holds for $x > x^*$. Then starting from any $x_0 \in I$ the sequence defined by the iteration $x_{n+1} = f(x_n)$ converges to the fixed point x^*.*

PROOF:

If $x_0 = x^*$, then $x_n = x^*$ for all n, hence the statement is obviously true. If $x_0 < x^*$, then we show that $x_n < x^*$ for all n and the sequence is increasing, hence it converges to x^*. Namely, the strict monotonicity of f implies that $f(x) < x^*$ for all $x < x^*$, hence $x_n < x^*$ implies $x_{n+1} = f(x_n) < x^*$. Thus starting below the fixed point the whole sequence remains below the fixed point. On the other hand, $x_n > x^*$ yields $x_{n+1} = f(x_n) < x_n$, thus the sequence is decreasing in this case. If $x_0 > x^*$, then it can be shown similarly that $x_n > x^*$ for all n and the sequence is decreasing, hence it converges to x^*.
□

Applying the Lemma, we will show below that starting from any $x_0 \in (0, N)$ the iteration $x_{n+1} = f(x_n)$ converges to the fixed point x^* guaranteed by Proposition 1 if it is unique, and to the positive fixed point if $S_0 = N$ and $\tau n > \gamma$.

Proposition 2 *Let x^* be the fixed point of the function $f(x) = N - S_0 e^{-Bx}$ in the interval $[0, N]$ if $S_0 \in [0, N)$ or $S_0 = N$ and $\tau n \leq \gamma$, and let x^* be the positive fixed point if $S_0 = N$ and $\tau n > \gamma$. Then for any $x_0 \in (0, N)$ the sequence defined by the iteration $x_{n+1} = f(x_n)$ converges to x^*.*

PROOF:

Let us start with the simpler case $S_0 = N$ and $\tau n \leq \gamma$ when $x^* = 0$. Then the concavity of the graph of f implies that it lies below the diagonal $y = x$, that is $f(x) < x$ holds for all positive x. Hence $x_{n+1} = f(x_n) < x_n$, i.e. the sequence is decreasing. On the other hand, x_n is non-negative for all n, therefore the sequence is convergent. The limit is obviously a fixed point of f, hence by the uniqueness of the fixed point x_n converges to $x^* = 0$. Let us turn now to the case when x^* is positive. The concavity of the graph of f implies that $f(x) > x$ in the left half of its domain $[0, x^*)$ and $f(x) < x$ in the right half $(x^*, N]$. Differentiating f shows directly that it is strictly increasing, hence according to Lemma 1 the sequence is convergent and its limit is the fixed point x^*.
□

3   The pairwise model

The second mean-field like approximation of SIR epidemic propagation on a homogeneous network is the so-called pairwise model. In this system differential equations are formulated not only for the number of nodes in different states but also for edges of different types. The system can be written in the following form [13].

$$[\dot{S}]_s = -\tau[SI]_s, \tag{5}$$

$$[\dot{I}]_s = \tau[SI]_s - \gamma[I]_s, \tag{6}$$

$$[\dot{R}]_s = \gamma[I]_s, \tag{7}$$

$$[\dot{SI}]_s = -(\tau + \gamma)[SI]_s + \tau\frac{n-1}{n}\frac{[SI]_s([SS]_s - [SI]_s)}{[S]_s}, \tag{8}$$

$$[\dot{SS}]_s = -2\tau\frac{n-1}{n}\frac{[SI]_s[SS]_s}{[S]_s}, \tag{9}$$

where $[S]_s(t)$, $[I]_s(t)$, $[R]_s(t)$, $[SI]_s(t)$, $[SS]_s(t)$ denote the pairwise approximation of the expected value of the number of susceptible, infected, recovered nodes, SI and SS edges at time t, respectively, the subscript "s" refers to "second" since this can be considered as the second approximation when the number of triples is expressed in terms of the number of pairs. The parameters τ and γ are again the per-contact infection rate and the recovery rate, n is the average degree of the network. We note that this system is derived from an exact model by approximating the triples in terms of the pairs as

$$[SSI] \sim \frac{n-1}{n}\frac{[SI][SS]}{[S]}, \quad [SII] \sim \frac{n-1}{n}\frac{[SI]^2}{[S]}.$$

It can again be easily seen that the first three differential equations are not independent since the conservation equation $[S]_s(t) + [I]_s(t) + [R]_s(t) = N$ holds, where N denotes the total number of nodes in the network. We are mainly interested in the final epidemic size $R_\infty = \lim\limits_{t \to \infty}[R]_s(t)$. We note that the proper notation would be R_∞^s, since this quantity is given by the second approximation and hence differs from the exact value of the final epidemic size. However, for the sake of simplicity we omit the superscript "s". The final epidemic size can be obtained from an implicit equation that can be derived from the differential equations, see e.g. [13]. Our goal with exploring this model is to prove the existence and uniqueness of the solution of this implicit equation and to show that simple iteration converges to the unique solution. For the Reader's convenience we also show a

simple derivation of the implicit equation in a slightly more direct way as it can be found in [13].

3.1 Derivation of the implicit equation for the final epidemic size

When there are no more infected individuals, the epidemic reaches completion, so we have $S_\infty + R_\infty = N$. We will derive an implicit equation for S_∞. For simplicity we assume $[R]_s(0) = 0$, so $[S]_s(0) + [I]_s(0) = N$ and we will use the initial conditions $[S]_s(0) = S_0$, $[I]_s(0) = N - S_0$, $[SS]_s(0) = \frac{S_0}{N}nS_0$ and $[SI]_s(0) = \frac{N-S_0}{N}nS_0$.

Substituting $[SI]$ from (5) into equation (9) yields

$$\frac{[\dot{SS}]_s}{[SS]_s} = 2\frac{n-1}{n}\frac{[\dot{S}]_s}{[S]_s}.$$

Using the initial conditions, integration leads to

$$[SS]_s = S_0^{\frac{2}{n}}\frac{n}{N}[S]_s^{\frac{2(n-1)}{n}}. \tag{10}$$

Now, substitute $[SI]$ from (5) and $[SS]$ from (10) into (8).

$$[\dot{SI}]_s - \frac{n-1}{n}\frac{[SI]_s}{[S]_s}[\dot{S}]_s = \frac{\tau+\gamma}{\tau}[\dot{S}]_s - \frac{n-1}{N}S_0^{\frac{2}{n}}[S]_s^{\frac{n-2}{n}}[\dot{S}]_s. \tag{11}$$

This linear differential equation can be solved by using the integrating factor $[S]_s^{\frac{1-n}{n}}$. Multiplying the equation by $[S]_s^{\frac{1-n}{n}}$ yields

$$\frac{\mathrm{d}}{\mathrm{d}t}\left([SI]_s[S]_s^{\frac{1-n}{n}}\right) = \frac{\tau+\gamma}{\tau}[S]^{\frac{1-n}{n}}[\dot{S}]_s - \frac{n-1}{N}S_0^{\frac{2}{n}}[S]^{\frac{-1}{n}}[\dot{S}]_s.$$

Integrating from $t = 0$ to $t = \infty$ and using that $[SI]_s(\infty) = 0$ leads to

$$-[SI]_s(0)S_0^{\frac{1-n}{n}} = \left[\frac{\tau+\gamma}{\tau}n[S]^{\frac{1}{n}}\right]_{S_0}^{S_\infty} - \left[\frac{n-1}{N}S_0^{\frac{2}{n}}\frac{n}{n-1}[S]^{\frac{n-1}{n}}\right]_{S_0}^{S_\infty}$$

After straightforward algebra and using the initial condition for $[SI]_s(0)$, we get

$$S_\infty^{\frac{2}{n}}N(\tau+\gamma) = S_\infty^{\frac{1}{n}}N\gamma S_0^{\frac{1}{n}} + S_\infty\tau S_0^{\frac{2}{n}}.$$

Equivalently, it can be written as:

$$S_\infty = S_\infty^{\frac{2}{n}}N\frac{\tau+\gamma}{\tau}S_0^{-\frac{2}{n}} - S_\infty^{\frac{1}{n}}N\frac{\gamma}{\tau}S_0^{-\frac{1}{n}}. \tag{12}$$

3.2 Uniqueness of the nontrivial solution of the implicit equation

Now our aim is to prove that (12) has a unique solution $S_\infty \in [0, N)$ for any $S_0 \in [0, N)$, yielding the positive final epidemic size as $R_\infty = N - S_\infty$. In the case when there are no infected nodes initially, i.e. $S_0 = N$, all nodes remain susceptible, that is we have the trivial solution $R_\infty = 0$. We note that it is interesting to investigate the limit of R_∞ as S_0/N tends to 1. If this limit is zero then we do not have epidemic with a small initial infection (i.e. with I_0/N tending to zero.) However, it may happen that the limit is positive,

meaning that even a very small initial infection can lead to a positive final epidemic size. Our derivation will yield the threshold value of the infection rate τ separating these two behaviours.

In order to prove the existence and uniqueness of the solution of (12), it is useful to introduce the new variable $y = S_\infty/S_0$, for which $y \in [0,1]$ holds, since $[S]$ is decreasing in time. For this variable $y = 0$ means that the entire population becomes infected and then removed during the epidemic, while $y = 1$ means that the disease dies out without causing any infection. Equation (12) takes the form $yS_0 = y^{2/n}N\frac{\tau+\gamma}{\tau} - y^{1/n}N\frac{\gamma}{\tau}$ for the new unknown y. This form is not suitable to prove the uniqueness and to apply the iteration hence the following transformations are carried out first to obtain a proper fixed point equation. Multiplying the equation by $\tau y^{1-2/n}$ and dividing by $N(\tau + \gamma)$ leads to

$$\frac{\tau S_0}{N(\tau+\gamma)}y^{2-\frac{2}{n}} + \frac{\gamma}{\tau+\gamma}y^{1-\frac{1}{n}} = y. \tag{13}$$

This is in the form of a fixed point equation $g(y) = y$ with

$$g(y) = Ay^{2q} + By^q, \quad \text{where } A = \frac{\tau}{\tau+\gamma}\frac{S_0}{N}, \quad B = \frac{\gamma}{\tau+\gamma}, \quad q = 1 - \frac{1}{n}.$$

Further, we assume that the network contains no isolated nodes and it is connected, hence for the average degree $n > 1$ holds, implying $0 < q < 1$.

Now our aim is to find the fixed point $y^* \in [0,1]$ of g. Then $S_\infty = S_0y^*$ and the final epidemic size is given as $R_\infty = N - S_0y^*$. Since $g(0) = 0$ we have zero as a fixed point corresponding to $R_\infty = N$, which occurs only in the case when we start from a totally infected population. In what follows, we will disregard this trivial case and look for the fixed point of g in $(0,1]$. We note that $y^* = 1$ corresponds to the other extreme case $R_\infty = 0$ when there is no epidemic at all. This can happen only in the case when $S_0 = N$, i.e. starting from a totally susceptible population. Concerning the fixed points of g we will need the following elementary statement.

Lemma 2 *Let $h : [0,1] \to \mathbb{R}$ be a twice differentiable function satisfying $h(0) = 0$, $h(1) \le 0$ and $h'(0) > 0$ (allowing also $h'(0) = +\infty$, which means that the right hand side limit of h' at 0 is infinity). If h has at least two zeros in $(0,1)$, then h'' also has at least two zeros in $(0,1)$.*

PROOF: We will make use of Rolle's theorem, according to which the derivative of a differentiable function has a zero between two zeros of the function. Applying Rolle's theorem to h' we get that h'' has at least two zeros if h' has at least three zeros, hence this latter statement is enough to prove. Let the two zeros of h in $(0,1)$ be $z_1 < z_2$. If h has a third zero in $(0,1)$ then there are four zeros of h together with 0. Hence according to Rolle's theorem, the derivative h' has at least three zeros between the four zeros of h, leading to the desired statement. Thus we need to prove the statement only in the case when h has exactly two zeros in $(0,1)$. We prove in the case when $h(1) < 0$, the proof is similar in the case $h(1) = 0$. Since h has only two zeros and using the sign conditions at the end points of the interval we have that $h(y)$ is positive in $(0, z_1)$ and negative in $(z_2, 1)$. Moreover, h does not change sign in (z_1, z_2), so it is either positive or negative in that interval. If it is positive there, then it has a local minimum at z_1, hence $h'(z_1) = 0$. Moreover, h is positive in the intervals $(0, z_1)$ and (z_1, z_2) and it is zero at the end points of these intervals, therefore it has local maxima inside these intervals, where h' is zero.

Thus h' has at least three zeros in $(0,1)$ that we wanted to prove. If h is negative in the interval (z_1, z_2), then similar reasoning leads to the desired existence of the three zeros of h'.
□

Returning to the fixed points of g we can prove the following result.

Proposition 3 *If $S_0 < N$, then g has a unique fixed point in $y^* \in (0,1)$, moreover $g(y) > y$ in $(0, y^*)$ and $g(y) < y$ in $(y^*, 1)$. If $S_0 = N$, then $y^* = 1$ is a fixed point. If $S_0 = N$ and $\tau(n-2) > \gamma$, then g has another unique fixed point in $(0,1)$, while for $\tau(n-2) \leq \gamma$ only the trivial fixed point exists and $g(y) > y$ holds in $(0,1)$.*

PROOF: Since $q < 1$ the graph of g has a vertical tangent at $y = 0$ (i.e. $g'(0) = +\infty$), thus we have $g(y) > y$ for small positive values of y. On the other hand, $g(1) = A + B = \frac{\tau}{\tau+\gamma}\frac{S_0}{N} + \frac{\gamma}{\tau+\gamma} \leq 1$ and $g(1) = 1$ if and only if $S_0 = N$. Thus the continuity of g implies that its graph intersects the diagonal straight line connecting the points $(0,0)$ and $(1,1)$, that is a fixed point exists in $(0,1)$ if $S_0 < N$. For the uniqueness of the fixed point let us investigate the convexity of g. Differentiating g twice, we get after simple algebra that

$$g''(y) = 2q(2q-1)Ay^{2q-2} + Bq(q-1)y^{q-2} = \frac{n-1}{n^2(\tau+\gamma)}y^{q-2}\left(\frac{2S_0}{N}(n-2)\tau y^q - \gamma\right).$$

One can see that the right hand side is either negative for all $y \in (0,1)$, i.e. g is concave in the interval $(0,1)$, or it has a single zero $\overline{y} \in (0,1)$, meaning that g is concave in $(0,\overline{y})$ and convex in $(\overline{y}, 1)$. The existence of two fixed points in $(0,1)$ is excluded by Lemma 2. Thus the existence of a unique fixed point in $(0,1)$ is proved for $S_0 < N$.

Let us turn to the case $S_0 = N$, when we have $g(1) = 1$ and $g'(1) = \frac{(n-1)(2\tau+\gamma)}{n(\tau+\gamma)} = 1 + \frac{\tau(n-2)-\gamma}{n(\tau+\gamma)}$. That is 1 is a fixed point and the existence of another fixed point depends on $g'(1)$. Namely, if $g'(1) > 1$, then the graph of $g(y)$ is below the diagonal for y close to 1, hence there is a fixed point in $(0,1)$. The uniqueness of the fixed point follows again from Lemma 2 based on the fact that g can have at most one inflection point. Thus, for $\tau(n-2) > \gamma$ we have $g'(1) > 1$, and there is a unique fixed point in $(0,1)$. If $\tau(n-2) \leq \gamma$ then $g'(1) \leq 1$. Hence, g has no fixed point in $(0,1)$. That can be proved again by using the fact that g can have at most one inflection point.
□

3.3 Solving the implicit equation numerically by iteration

Now we show how the solution of (12) can be found by using an iteration. First, the fixed point $y^* \in [0,1]$ of g is determined by using the iteration $y_{n+1} = g(y_n)$. Then $S_\infty = S_0 y^*$ and the final epidemic size is given as $R_\infty = N - S_0 y^*$.

Proposition 4 *Let $y^* \in (0,1)$ be the unique fixed point of the function g if $S_0 < N$ or $S_0 = N$ and $\tau(n-2) > \gamma$, and let $y^* = 1$ if $S_0 = N$ and $\tau(n-2) \leq \gamma$. Then for any $y_0 \in (0,1)$ the sequence defined by the iteration $y_{n+1} = g(y_n)$ converges to y^*.*

PROOF:

Differentiating g we get $g'(y) = 2qAy^{2q-1} + qBy^{q-1} > 0$, hence g is strictly increasing. According to Proposition 3 the function g satisfies the conditions of Lemma 1, and therefore the sequence given by $y_{n+1} = g(y_n)$ converges to y^*.
□

4 Heterogeneous mean-field model

Let us now turn to the case of heterogeneous networks, i.e. when there are nodes with different degrees. Let N_k denote the number of nodes of degree k, then $N_1 + N_2 + N_3 + \ldots + N_K = N$ with K being the highest degree. The expected value of the number of susceptible, infected and recovered nodes of degree k at time t are denoted by $[S_k](t)$, $[I_k](t)$ and $[R_k](t)$, respectively. The variables are related by the equation $[S_k](t) + [I_k](t) + [R_k](t) = N_k$ for any degree k and satisfy the set of differential equations [19]

$$[\dot{S}_k] = -\tau[S_kI], \tag{14}$$

$$[\dot{I}_k] = \tau[S_kI] - \gamma[I_k], \tag{15}$$

$$[\dot{R}_k] = \gamma[I_k], \tag{16}$$

where $[S_kI]$ denotes the expected number of edges connecting susceptible nodes of degree k to infected nodes (of any degree). This system is not self-contained, the pairs need to be expressed in terms of the singles. This is based on the approximation $[S_kI] \approx kQ[S_k]$, where $Q = \frac{\sum j[I_j]}{\sum jN_j}$ represents the probability that an edge starting from a given node is linked to an infected node [19]. Using this approximation the following self-contained system of ODEs can be obtained [19].

$$[\dot{S}_k]_a = -\tau k[S_k]_aQ_a, \tag{17}$$

$$[\dot{I}_k]_a = \tau k[S_k]_aQ_a - \gamma[I_k]_a, \tag{18}$$

$$[\dot{R}_k]_a = \gamma[I_k]_a, \tag{19}$$

$$Q_a = \frac{\sum j[I_j]_a}{\sum jN_j}. \tag{20}$$

The subscript "a" refers to the fact that these variables are approximations of the corresponding exact quantities. Our aim is to investigate the final epidemic size given by this heterogeneous mean-field approximation. We note that networks with heterogeneous degree distribution can also be modeled by the edge based compartmental model [17, 23] and the household structure can also be taken into account [10].

4.1 Derivation of the implicit equation for the final epidemic size

Similarly to the homogeneous mean-field system, the epidemic propagation stops when there are no more infected individuals, so we have again $[S_k]_a(\infty) + [R_k]_a(\infty) = N_k$. For simplicity we assume $[R_k]_a(0) = 0$, so $[S_k]_a(0) + [I_k]_a(0) = N_k$. We can rewrite equation (17) as $[\dot{S}_k]_a + \tau k[S_k]_a d\sum j[I_j]_a = 0$ with $d = 1/\sum jN_j$. Based on (19) this can be written as

$$[\dot{S}_k]_a + \frac{\tau kd}{\gamma}[S_k]_a \sum j[\dot{R}_j]_a = 0.$$

Using the integrating factor $\exp\left(\frac{\tau kd}{\gamma}\sum j[R_j]_a\right)$ we get

$$\frac{\mathrm{d}}{\mathrm{d}t}\left([S_k]_a \exp\left(\frac{\tau kd}{\gamma}\sum j[R_j]_a\right)\right) = 0.$$

Integrating this from 0 to ∞ and using $[R_k]_a(0) = 0$ leads to

$$[S_k]_a(\infty) = [S_k]_a(0)\Theta^k, \quad \text{with} \quad \Theta = \exp\left(-\frac{\tau kd}{\gamma}\sum j[R_j]_a(\infty)\right)$$

yielding the final epidemic size

$$[R_k]_a(\infty) = N_k - [S_k]_a(0)\Theta^k. \tag{21}$$

Now, we need to determine Θ as the solution of a fixed point equation. In order to derive this equation, multiply (21) by k, sum for all k, then multiply by $-\tau k d/\gamma$ and finally take its exponential. These operations yield Θ in the left hand side and lead to the fixed point equation

$$\Theta = f(\Theta) \quad \text{with} \quad f(x) = \exp\left(-\frac{\tau}{\gamma} + \frac{\tau d}{\gamma}\sum k[S_k]_a(0)x^k\right). \tag{22}$$

4.2 Uniqueness of the solution of the implicit equation

Let $S_0 = \sum[S_j]_a(0)$ denote the total number of susceptible nodes at $t = 0$. Now our aim is to prove that (22) has a unique solution $\Theta \in (0, 1)$ for any $S_0 \in [0, N)$, yielding the positive final epidemic size among degree k nodes by (21) and the total final epidemic size as $R_\infty = \sum[R_k]_a(\infty)$. In the case when there are no infected nodes initially, i.e. $S_0 = N$, all nodes remain susceptible, that is we have the trivial solution $R_\infty = 0$. We note that it is interesting to investigate the limit of R_∞ as S_0/N tends to 1. If this limit is zero then we do not have epidemic with a small initial infection (i.e. with I_0/N tending to zero.) However, it may happen that the limit is positive, meaning that even a very small initial infection can lead to a positive final epidemic size. Our derivation will yield the threshold value of the infection rate τ separating these two behaviours.

Proposition 5 *Let* $\langle K \rangle = \sum k N_k/N$ *and* $\langle K^2 \rangle = \sum k^2 N_k/N$ *be the first and second moments of the degree distribution. If* $S_0 < N$, *then* f *has a unique fixed point* $\Theta^* \in (0, 1)$, *moreover* $f(\Theta) > \Theta$ *in* $(0, \Theta^*)$ *and* $f(\Theta) < \Theta$ *in* $(\Theta^*, 1)$. *If* $S_0 = N$, *then* $\Theta^* = 1$ *is a fixed point. If* $S_0 = N$ *and* $\tau\langle K^2 \rangle > \gamma\langle K \rangle$, *then* f *has another unique fixed point in* $(0, 1)$, *while for* $\tau\langle K^2 \rangle \le \gamma\langle K \rangle$ *only the trivial fixed point exists and* $f(\Theta) > \Theta$ *holds in* $(0, 1)$.

PROOF:
We have $f(0) = \exp(-\tau/\gamma) > 0$ and

$$f(1) = \exp\left(\frac{\tau}{\gamma}\left(\frac{\sum k[S_k]_a(0)}{\sum k N_k} - 1\right)\right) \le 1$$

since $[S_k]_a(0) \le N_k$ for all k. If $S_0 < N$, then there exist at least one value of k, for which $[S_k]_a(0) < N_k$ holds, hence $f(1) < 1$, while for $S_0 = N$ we have $[S_k]_a(0) = N_k$ for all k yielding $f(1) = 1$. Thus, in the case $S_0 < N$, the continuity of f implies that its graph intersects the diagonal (the line segment connecting the points $(0, 0)$ and $(1, 1)$), hence the existence of a fixed point $\Theta^* \in (0, 1)$ follows. In order to prove its uniqueness let us calculate the second derivative of f. It can be written in the form $f(x) = \exp(p(x))$, where p is a polynomial with positive coefficients (except the constant term). Hence $p'' > 0$ and the second derivative of f satisfies $f'' = \exp(p)(p'^2 + p'') > 0$, that is f is convex in the interval $(0, 1)$. Since its graph starts above and ends below the diagonal, it has a unique intersection point with the diagonal. Thus we have $f(\Theta) > \Theta$ in $(0, \Theta^*)$ and $f(\Theta) < \Theta$ in $(\Theta^*, 1)$.

Let us turn to the case $S_0 = N$. In this case we have $f(1) = 1$, hence 1 is a fixed point. The convexity of the graph implies that the existence of a fixed point in the open interval $(0, 1)$ depends on $f'(1)$. If $f'(1) > 1$, then $f(\Theta)$ is below the diagonal when Θ is close to 1,

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hence by the continuity of f it has a fixed point in the open interval $(0, 1)$. For $f'(1) \leq 1$ the graph of f is above the diagonal, i.e. $f(\Theta) > \Theta$ holds in $(0, 1)$. Differentiating f shows

$$f'(1) = \frac{\tau \langle K^2 \rangle}{\gamma \langle K \rangle}$$

proving the desired statement.
□

4.3 Solving the implicit equation numerically by iteration

Now we show how can the final epidemic size be determined by using an iteration. First, the fixed point $\Theta^* \in (0, 1]$ of f is determined by using the iteration $\Theta_{n+1} = f(\Theta_n)$. Then the final epidemic size among degree k nodes is given by (21) and the total final epidemic size is

$$R_\infty = N - \sum [S_k]_a(0)(\Theta^*)^k.$$

Proposition 6 *Let $\Theta^* \in (0, 1)$ be the unique fixed point of the function f if $S_0 < N$ or $S_0 = N$ and $\tau \langle K^2 \rangle > \gamma \langle K \rangle$, and let $\Theta^* = 1$ if $S_0 = N$ and $\tau \langle K^2 \rangle \leq \gamma \langle K \rangle$. Then for any $\Theta_0 \in (0, 1)$ the sequence defined by the iteration $\Theta_{n+1} = f(\Theta_n)$ converges to Θ^*.*

PROOF:

Differentiating f shows that f is strictly increasing. According to Proposition 5 the function f satisfies the conditions of Lemma 1, therefore the sequence given by $\Theta_{n+1} = f(\Theta_n)$ converges to Θ^*.
□

5 Comparison of the final epidemic size obtained from the stochastic and the mean-field ODE models

The final epidemic size, together with the epidemic distribution, can be obtained from the exact stochastic model for graphs with special structure. We derive the epidemic distribution and the mean final size for the line, the star and the complete graphs below. The derivation strongly exploits the special structure of these graphs, and hence the exact value of the final epidemic size is not available in general. As an alternative, the final epidemic size can be obtained from different mean-field type approximations. In Sections 2, 3 and 4 it was determined for the homogeneous mean-field, homogeneous pairwise and heterogeneous mean-field models. These approximations are supposed to perform well for random graphs, or for the complete graph. Therefore, a comparison to the exact stochastic model will be carried out only for the complete graph, which is dealt with in the second part of this section.

5.1 Final size distribution for Markovian SIR epidemic

Epidemic propagation on a network can be modeled by a continuous time Markov chain under the assumption of memorylessness, i.e. assuming exponentially distributed times between events. Since each node can be in one of the three states, susceptible, infected or recovered, the whole network has 3^N states, where N is the number of nodes. There can be two types of transitions between these states: a node recovers with rate γ, or

a susceptible node becomes infected with rate $i\tau$, where i is the number of its infected neighbours. Then the time evolution of the system is fully described by a system of linear ordinary differential equations, called master equations (or Kolmogorov forward equations), in which the unknowns are the probabilities of the states. Due to its large size, this system is hardly treatable, but for networks with special structure the final epidemic size distribution can be given analytically. During a SIR epidemic the number of infected nodes becomes zero at some time either because the infection is not strong enough or by the depletion of susceptible nodes. At that time the process finishes since further transitions cannot occur. The final epidemic size distribution is a probability distribution, p_k, yielding the probability that the number of recovered nodes on a given network is k when the epidemic is finished. From this we can find the mean final epidemic size as the expected value of $R_\infty = \sum_{k=1}^{N} k p_k$.

Based on the early work of Ludwig [14], it is possible to associate to a continuous time epidemic process another representation in discrete-time steps that has the same final size distribution, see [20]. This approach is often referred to as generation-based or rank-based description of the epidemic. Using this representation enables us to explicitly determine the final epidemic size distribution on small networks, or networks with special structure. We illustrate this first with the simplest example, a network with two nodes, i.e. a single edge. Let one node be infected and the other one be susceptible at the initial instant, represented by the state IS. The next event can be either infection, leading to the state II, or recovery, leading to RS. The probabilities of these transitions are $\tau/(\tau + \gamma)$ and $\gamma/(\tau+\gamma)$, respectively. The final epidemic size can be either 1, when the final state is RS, with probability $\gamma/(\tau + \gamma)$, or it can be two, when the final state is RR, with probability $\tau/(\tau + \gamma)$. Thus the final size distribution is $p_1 = \gamma/(\tau + \gamma)$, $p_2 = \tau/(\tau + \gamma)$. It can be immediately seen that this is a probability distribution because $p_1 + p_2 = 1$.

As this simple example shows, the time dependence of the process is not considered in the course of this approach. The calculations can be carried out especially easily if at each step there is a single infected node that can transmit infection. Then two events can happen: either this node infects one of its neighbours or it recovers. In these cases the probability of infection is

$$x_i = \frac{i\tau}{i\tau + \gamma} \tag{23}$$

and the probability of recovery is $1 - x_i = \frac{\gamma}{i\tau+\gamma}$, where i is the number of susceptible neighbours.

Below we determine the final epidemic size distribution by using the rank-based approach for three special network types: the line, the star and the complete graphs. These graphs can be recursively defined by the number of nodes. Our goal here is to find a recursive function yielding the final epidemic size for the line and the star graphs. For a given network, let $P_{K,k}$ be the probability of having k recovered nodes on a K node graph when the epidemic is finished.

5.1.1 Final epidemic size distribution for the line graph

One notable example of a recursion is a line graph with the initial infected node at one of its endpoints, denoted as $ISS\ldots S$. The case of an edge ($K = 2$) dealt with above is a special case. For $K = 2$ we saw that $P_{2,1} = 1 - x_1$, $P_{2,2} = x_1$. Let us consider now the case $K = 3$, i.e. a line graph on three nodes with one infected node at the end. This state can be represented as ISS. Then the node on the end can recover, leading to the state RSS,

with probability $p_1 = 1 - x_1$. (Note that x_i is given in (23).) If the node infects the adjacent node, leading to the state IIS, then the node on the end can't interact with anything, so we can consider that node removed. Again, the infected node in the middle can recover, with probability $p_2 = x_1(1 - x_1)$, or alternatively, the infected node can infect the last remaining adjacent node, with probability $p_3 = x_1^2$. Thus the final state can be RSS with probability p_1, RRS with probability p_2 and RRR with probability p_3, thus the final size distribution is determined. We can easily see that $p_1 + p_2 + p_3 = 1 - x_1 + x_1(1 - x_1) + x_1^2 = 1$. Thus for $K = 3$ we have $P_{3,1} = 1 - x_1$, $P_{3,2} = x_1(1 - x_1)$ and $P_{3,3} = x_1^2$. The mean final epidemic size is

$$R_\infty = p_1 + 2p_2 + 3p_3 = 1 + x_1 + x_1^2.$$

We note that a line graph on three nodes but with the infected node in the middle can be considered similarly, leading to $p_1 = 1 - x_2$, $p_2 = x_2(1 - x_1)$, $p_3 = x_1 x_2$ and final epidemic size

$$R_\infty = p_1 + 2p_2 + 3p_3 = 1 + x_2 + x_1 x_2.$$

It can be immediately seen that this final epidemic size is greater than the previous one corresponding to the case when the infection started at the end point.

Turning to the case of a line graph with arbitrary length, note that since the infection can only move one way and thus isolate the other infected nodes, if an I infects an adjacent node the previous node cannot interact with the rest of the graph; so we can consider that point removed. So if we have a path with K nodes, the node on the end can go to R, thus $P_{K,1} = 1 - x_1$. If the node infects the adjacent node then the node on the end can't interact with anything, so we can consider that node removed by default.

Now observe that $P_{K,2} = x_1 P_{K-1,1}$ since the probability of an infection is x_1 and now we are recalculating the probability for an I going to an R on the end of a $K - 1$ path. We can follow this reasoning down the path to obtain that $P_{K,k} = x_1 P_{K-1,k-1} = x_1^2 P_{K-2,k-2} = \cdots = x_1^{k-1} P_{K-k+1,1} = x_1^{k-1}(1 - x_1)$, which holds for $k = 1, 2, \ldots, K - 1$. Note that $P_{1,1} = 1$, leading to $P_{2,2} = x_1$ and, in general, $P_{K,K} = x_1^{K-1}$. Summarizing we get the following statement for the line graph:

Proposition 7 *Starting the infection from the end point of a line graph of length K, the probability $P_{K,k}$ of having k recovered nodes when the epidemic finishes is*

$$P_{K,k} = x^{k-1}(1 - x_1) \quad for \quad k \in \{1, 2, \ldots, K - 1\} \quad and \quad P_{K,K} = x_1^{K-1}.$$

This is a probability distribution, that is $\sum_{i=1}^{K} P_{K,i} = 1$ and the expected value of the number of recovered nodes, i.e. the final epidemic size, is

$$R_\infty = 1 + x_1 + x_1^2 + \ldots + x_1^{K-1}.$$

Only the final epidemic size formula needs verification. It follows from $R_\infty = \sum_{i=1}^{K} i P_{K,i}$ after simple algebra.

5.1.2 Final epidemic size distribution for a star graph

The K node star graph is a tree where one node has degree $K - 1$ and the rest of the nodes have degree one. This recursion is for one infected node at the highest degree on a K node star graph. Note that the initial I node is adjacent to $K - 1$ S nodes. What can happen first is that the I node can to go R, thus stopping the spread of infection, leading to $P_{K,1} = 1 - x_{K-1}$. (Note that x_i is given in (23).)

However if an adjacent node is infected, we get a leaf with an infected node at the end. Since this leaf is not connected to anything, we can say that node is removed and we are left calculating a recursion for a $K-1$ node star graph. Note that once we have an R on a leaf, that is one less node for the subsequent recursions.

Now observe that $P_{K,2} = x_{K-1}P_{K-1,1}$. We can use this same reasoning to get the recursive relation $P_{K,k} = x_{K-1}P_{K-1,k-1}$. Applying this formula iteratively yields

$$P_{K,k} = x_{K-1}P_{K-1,k-1} = x_{K-1}x_{K-2}P_{K-2,k-2} = \dots$$

$$= \prod_{i=K-k+1}^{K-1} x_i P_{K-k+1,1} = (1 - x_{K-k}) \prod_{i=K-k+1}^{K-1} x_i,$$

which holds for $k = 2, \dots, K-1$. Starting from $P_{1,1} = 1$ and applying the recursion $P_{K,k} = x_{K-1}P_{K-1,k-1}$ we get $P_{K,K} = \prod_{i=1}^{K-1} x_i$. Summarizing we get the following statement for the star graph:

Proposition 8 *Starting the infection from the central node of a star graph with K nodes, the probability $P_{K,k}$ of having k recovered nodes when the epidemic finishes is*

$$P_{K,1} = 1 - x_{K-1}, \quad P_{K,k} = (1 - x_{K-k}) \prod_{i=K-k+1}^{K-1} x_i \quad \text{for } k \in \{2, \dots, K-1\}, \quad P_{K,K} = \prod_{i=1}^{K-1} x_i.$$

This is a probability distribution, that is $\sum_{i=1}^{K} P_{K,i} = 1$ and the expected value of the number of recovered nodes, i.e. the final epidemic size, is

$$R_\infty = 1 + x_{K-1} + x_{K-2}x_{K-1} + x_{K-3}x_{K-2}x_{K-1} + \dots + x_1 x_2 \dots x_{K-1}.$$

Only the final epidemic size formula needs verification. It follows from $R_\infty = \sum_{i=1}^{K} iP_{K,i}$ after simple algebra. The formula for the final epidemic size can easily be compared to that of belonging to the line graph given in Proposition 7. Namely, the inequality $x_1 < x_i$ implies that the final epidemic size for the star is greater than that of the line graph.

5.1.3 Final epidemic size distribution for the complete graph

Let us start with a triangle with one infected node, represented again by SIS, but in this case the two susceptible nodes are neighbours. The infected node can recover, leading to the state SRS, with probability $p_1 = 1 - x_2$ since it has two susceptible neighbours. If the node infects one of the adjacent nodes with probability x_2, leading to the state IIS, then both infected nodes can infect the susceptible one. If both of them recovers before transmitting infection, then the triangle arrives to the state RRS, this happens with probability $p_2 = x_2(1 - x_1)^2$. On the other hand, the last node can be infected making all nodes removed. There are two ways this can happen, one way is to have an I infecting the S and the other way is to have one I become an R and then the other I infects the susceptible node. So we therefore have $p_3 = x_2x_1(1 - x_1) + x_2x_1$. We can check that $p_1 + p_2 + p_3 = 1 - x_2 + x_2(1 - x_1)^2 + x_2x_1(1 - x_1) + x_2x_1 = 1$. The final epidemic size is

$$R_\infty = p_1 + 2p_2 + 3p_3 = 1 + x_2(4 - x_1 - x_1^2).$$

Simple calculation shows that $1 + x_1 \le 4 - x_1 - x_1^2$, hence this final epidemic size is greater than the one corresponding to the case of a line graph with infection starting from the middle point.

The case of a complete graph with arbitrary size is more complicated than those of the line and the star graphs. While we will not go into detail, we will provide a brief illustration for a recent result of an iterative method for the epidemic size distribution of the complete graph developed by Black and Ross [11]. The intuition is that the epidemic process can be considered as a random walk that end in an absorbing state that determines the final size distribution. They mention that it can be difficult to enumerate all the paths and correctly sum them because it is hard to determine whether all relevant terms are included.

They manage to solve this problem with *degree-of-advancement* (DA) representation. It is based on counting events instead of population numbers and a lexicographical ordering of the state space [11]. The state space itself is the possible walks that are available to the complete graph. The state of the process is represented by the pair (S, I), which is the number of susceptible and infected individuals at a given time step. Two transitions are possible: infection, represented by $(S, I) \rightarrow (S - 1, I + 1)$, with rate $\tau S I$, and recovery, represented by $(S, I) \rightarrow (S, I - 1)$ with rate γI.

In contrast they count the number of events rather than the population, so they define a new vector (Z_1, Z_2) to represent the number of infection and recovery events, respectively. The initial condition of the problem is set up by $Z_1 = I_0$, $Z_2 = 0$, meaning that there are I_0 infected, $N - I_0$ susceptible and 0 recovered nodes when the process starts. The pair (Z_1, Z_2) is easier to work with since their values only increase by one at each step, while for (S, I) the numbers can increase or decrease along with the population. We can relate the number of susceptible, infected and recovered individuals to (Z_1, Z_2) by,

$$S = N - Z_1, \ I = Z_1 - Z_2, \ R = Z_2.$$

Using these relations the rates of each type of transition can be calculated in terms of Z_1 and Z_2. This way the process can be easily represented as a random walk on a two-dimensional lattice, and the probability of arriving to the different absorbing states can be determined by a simple iteration. Due to its simplicity, the algorithm can be applied for very large graphs as well. Unfortunately analytic formulas are not given in [11] for the final size distribution, the numerical results will be presented in Section 5.2.

5.2 Comparison of mean-field and stochastic models for the complete graph

Since the complete graph is regular, we use the homogeneous mean-field and pairwise approximations. The comparison is carried out for systems of various sizes and with different infection rates. For the comparison, the number of initially infected nodes has to be chosen carefully. If it is too small then the process may stop after a few infections and the mean-field approximation cannot perform well. Hence we assume that the process starts with at least 1% of the nodes initially infected.

The first analysis we performed considered how the mean-field approximations compare to the exact stochastic model as the value of the infection rate τ is varied, with a fixed value of the recovery rate, $\gamma = 1$. Using the algorithm developed by Black and Ross [11] and coded in Matlab, we determined the final epidemic size (measured by R_∞, the limit of the number of removed nodes as time approached infinity) from the exact stochastic model for several values τ. The final epidemic size was determined for the same values of τ from the homogeneous mean-field given by (4) using the iteration in Proposition 2. Similarly, using the iteration in Proposition 6, the final epidemic size is determined from

the homogeneous pairwise model as $R_\infty = N - S_\infty$ with S_∞ being the solution of (12). The comparison is shown in Figure 1 for a complete graph with $N = 1000$ nodes varying τ from 0 to 0.005.
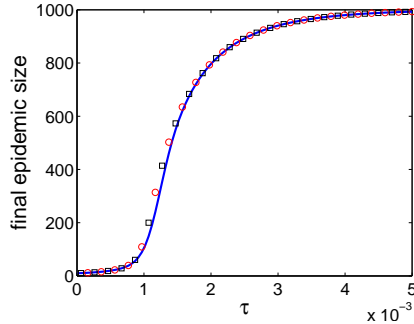

Figure 1: Final epidemic size for a complete graph with $N = 1000$ nodes for τ values varied between zero and 0.005 and for $\gamma = 1$ from the exact stochastic model (continuous blue curve), from the homogeneous mean-field approximation (red circles) and from the homogeneous pairwise model (black squares).

In order to study the accuracy of the mean field approximations, the relative error of the epidemic size is plotted. The relative error is defined as $(R_\infty^{mf} - R_\infty^{stoch})/R_\infty^{stoch}$, where R_∞^{mf} and R_∞^{stoch} are the final epidemic sizes obtained from the homogeneous mean-field model and from the exact stochastic model, respectively. The relative error for the pairwise model is defined similarly with R_∞^{pw} instead of R_∞^{mf}. The relative errors of the mean-field and pairwise approximations are shown in Figure 2 for a complete graph with $N = 1000$ nodes varying τ from 0 to 0.005.
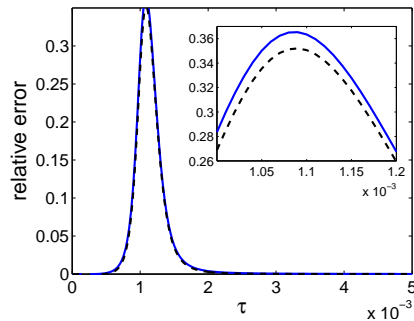

Figure 2: Relative errors of the mean-field (blue continuous curve) and pairwise (black dashed curve) approximations for a complete graph with $N = 1000$ nodes for τ values varied between zero and 0.005 and for $\gamma = 1$. The inset shows an enlarged part of the domain.

The analysis shows that the relative error becomes large (nearly 40%) when τ is close to its critical value $\tau_{crit} = \gamma/N$ obtained from the mean-field approximation given in Proposition 1. The reason that the approximations have spikes in accuracy as τ nears its critical value, can be explained by inspecting the final size distributions for different values of τ shown in Figure 3. This Figure shows that the distribution is unimodal, having a single maximum, if τ is not close to its critical value and this maximum is close

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to the expected value, i.e. the final epidemic size. However, for τ values close to the critical value the distribution is bimodal, hence the final epidemic size is between the two maxima. The mean-field and pairwise approximations fail to predict the final epidemic size for such distributions since the derivation of mean-field models is based on the fact that the distribution is concentrated around its expected value. We note that this phenomenon is less significant when there are more infected nodes initially.
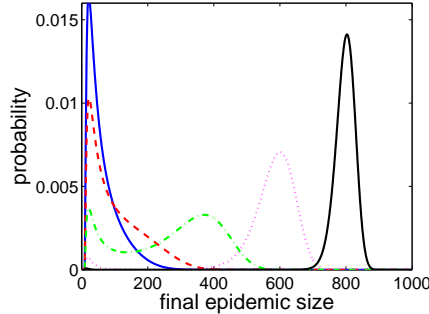

Figure 3: Final epidemic size distribution for a complete graph with $N = 1000$ nodes for different values of τ and $\gamma = 1$. $\tau = 0.9\tau_{crit}$ blue continuous curve, $\tau = \tau_{crit}$ red dashed curve, $\tau = 1.2\tau_{crit}$ green dashed-dotted curve, $\tau = 1.5\tau_{crit}$ pink dotted curve and $\tau = 2\tau_{crit}$ black continuous curve, where $\tau_{crit} = \gamma/N$ is the critical value of τ in the homogeneous mean-field model.

Another observation, shown by the inset in Figure 2, is that the pairwise approximation appears to have consistently lower relative error than the mean-field approximation, which indicates its better accuracy as a model.

To further examine the accuracy of the approximations as the size of the graphs increases, we determined the relative errors as the size of the graph is varied from $N = 200$ to $N = 1000$ and τ is a given multiple of its critical value $\tau_{crit} = \gamma/N$. (The number of initially infected nodes is 2% of the graph size). Figure 4 reaffirms how the accuracy of the pairwise approximation compares to the mean-field approximation. As the size of the graph increases the comparisons' R_∞ both converge to the exact stochastic model's solution for R_∞.
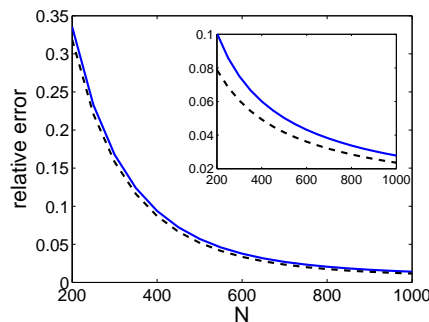

Figure 4: Relative error of the mean-field (blue continuous curve) and the pairwise (black dashed curve) approximations as the size of the complete graph is varied. The value of the infection rate is $\tau = 1.5\tau_{crit}$ in the main figure and $\tau = 0.8\tau_{crit}$ in the inset, the recovery rate is $\gamma = 3$ for both.

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It is clear from Figure 4 that the relative error in the approximations decreases as the size of the graph grows. The infection rate changes proportionally to the size of the graph (i.e. τ is proportional to $\tau_{crit} = \gamma/N$). While we have no formal proof, we conjecture that there is an inverse relationship between the relative error and size of the graphs as given by: $(R_\infty^{mf} - R_\infty^{stoch})/R_\infty^{stoch} \approx O(\frac{1}{N})$ and similarly for the relative error of the pairwise approximation.

6 Conclusion

We studied the final epidemic distribution and final epidemic size of an SIR epidemic for the line, star and complete graphs by using the exact stochastic models and the final epidemic size, R_∞, for the mean-field and pairwise approximations. In the case of the stochastic model the final size distribution was determined analytically for the above network types. For the mean-field and pairwise models, the implicit equations and their solutions for R_∞ were known. We proved the existence and uniqueness of such R_∞ values for both models, moreover we verified that a suitably chosen iteration converges to the unique solution of the implicit equation. Results relating the stochastic and deterministic models were also presented. It was shown that the pairwise model yields a more accurate approximation, especially when the infection rate is close to its critical value, or in other words, when the basic reproductive ratio is close to one. Numerical evidence showed that the relative error of the mean-field and pairwise approximations is of order $1/N$ as the network size N is increased. For the heterogeneous mean-field model, we proved the existence and uniqueness of a solution to the implicit formula. However, further research is needed to investigate the accuracy of the results compared to known models such that for the star graph.

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