Optimal allocation of resources for suppressing epidemic spreading on networks

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(Received 28 February 2017; published 27 July 2017)

Efficient allocation of limited medical resources is crucial for controlling epidemic spreading on networks. Based on the susceptible-infected-susceptible model, we solve the optimization problem of how best to allocate the limited resources so as to minimize prevalence, providing that the curing rate of each node is positively correlated to its medical resource. By quenched mean-field theory and heterogeneous mean-field (HMF) theory, we prove that an epidemic outbreak will be suppressed to the greatest extent if the curing rate of each node is directly proportional to its degree, under which the effective infection rate λ has a maximal threshold $\lambda_c^{\rm opt} = 1/\langle k\rangle$, where $\langle k\rangle$ is the average degree of the underlying network. For a weak infection region ($\lambda \gtrsim \lambda_c^{\rm opt}$), we combine perturbation theory with the Lagrange multiplier method (LMM) to derive the analytical expression of optimal allocation of the curing rates and the corresponding minimized prevalence. For a general infection region ($\lambda > \lambda_c^{\rm opt}$), the high-dimensional optimization problem is converted into numerically solving low-dimensional nonlinear equations by the HMF theory and LMM. Counterintuitively, in the strong infection region the low-degree nodes should be allocated more medical resources than the high-degree nodes to minimize prevalence. Finally, we use simulated annealing to validate the theoretical results.

DOI: 10.1103/PhysRevE.96.012321

I. INTRODUCTION

A challenging problem in epidemiology is how best to allocate limited resources of treatment and vaccination so that they will be most effective in suppressing or reducing outbreaks of epidemics. This problem has been a subject of intense research in statistical physics and many other disciplines [1,2]. Inspired by the percolation theory, the simplest strategy is to randomly choose a fraction of nodes to immunize. However, random immunization is inefficient for heterogeneous networks. Later, many more effective immunization strategies were developed, ranging from global strategies such as targeted immunization based on node degree [3] or betweenness centrality [4], to local strategies such as acquaintance immunization [5] and (bias) random-walk immunization [6,7], and to some others in between [8]. Further improvements were made by graph partitioning [9] and optimization of the susceptible size [10]. In addition to degree heterogeneity, community structure has a major impact on disease immunity [11,12]. Recently, a message-passing approach was used to find an optimal set of nodes for immunization [13]. The immunization was mapped onto the optimal percolation problem [14]. Based on the idea of explosive percolation, an "explosive immunization" method has been proposed [15]. However, some diseases such as the common cold and influenza, which can be modeled by the susceptible-infected-susceptible (SIS) model [30], do not confer immunity, and individuals can be infected over and over again. Under those situations, one way to control the spread of the diseases is to reduce the risk of infection, such as by adaptive rewiring of the links incident to infected individuals [16], and the dynamical interplay between awareness and epidemic spreading [17].

An alternative way to control the epidemic spreading of SIS type is by designing an optimal strategy for distributing the limited medical resources so as to suppress the epidemic outbreak to the greatest extent, and to minimize the prevalence once the epidemic outbreak has happened. It is reasonable to assume the curing rate of each node is positively correlated to the medical resources allocated to it. Therefore, the optimal allocation of medical resources is equivalent to that of the curing rates. Assuming that the medical resources are limited, the average curing rate is thus considered to be fixed. This problem has been addressed as a constraint optimization problem in several previous works. When the curing rate can only be tuned in a fixed number of feasible values, this problem has been proved to be NP-complete [18]. Instead, when the curing rate can vary continuously in a given interval, some efficient algorithms have been developed for minimizing the threshold of epidemic outbreak [19,20] or the steady-state infection density [21].

In the present work, we theoretically solve the constraint optimization problem in both epidemic-free and endemic phases within the mean-field framework. On the one hand, we prove that an epidemic outbreak can be suppressed to the greatest extent when the curing rate of each node is directly proportional to its degree under which the epidemic threshold is maximized, that is, the inverse of the average degree of the underlying network. On the other hand, once the epidemic has broken out but is close to the threshold, we analytically show that the optimal curing rate should be adjusted in terms of the difference between the node degree and the average degree, and the distance to epidemic threshold. For the general infection region, the optimization problem can be simplified to solve three nonlinear equations. Some closely related works have studied the SIS model [22] and its metapopulation version

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[23] with the curing rate, $\mu_k \sim k^\alpha$, but there was no guarantee that such a power-law form would be the optimal one. In [24], the authors considered a simple heuristic strategy to control epidemic extinction, where the curing rate is directly proportional to the node degree. They showed that on any graph with a bounded degree, the extinction time is sublinear with the size of the network. Further improvement was made using a heuristic PAGERANK algorithm to allocate curing rates based on the initial condition of infected nodes [25]. The present study does not require any assumptions about the form of the curing rates with node degrees in advance except that the mean curing rate is assumed to be fixed due to the limited medical resources.

The rest of the paper is organized as follows. In Sec. II, we propose the constraint optimization problem based on the SIS model. The maximized epidemic threshold and the corresponding optimal allocation of curing rates are derived analytically in Sec. III. We present the theoretical treatment of the constraint optimization problem in Sec. IV for the weak infection region, and in Sec. V for the general infection region. In Sec. VI, we show numerical demonstrations for theoretical results. Finally, the main conclusions and perspective are addressed in Sec. VII.

II. PROBLEM PROPOSITION

To formulate our problem, we consider the SIS model on an undirected network of size N. The network is described by an adjacency matrix $\mathbb{A}$ whose entries are defined as $A_{ij} = 1$ if nodes i and j are connected, and $A_{ij} = 0$ otherwise. Each node is either susceptible or infected. A susceptible node i can be infected by its infective neighbor with an infection rate β, and an infected node i recovers with a nonvanishing curing rate μ_i. Here, we consider that the curing rate is allowed to vary from one node to another. In general, the more medical resources are available for node i, the larger μ_i is. Assuming that the total amount of medical resources is limited, the average curing rate is thus fixed, i.e.,

$$\langle \mu_i \rangle = \mu \quad \text{and} \quad \mu_i \geqslant 0, \ \forall\, i. \tag{1}$$

Our goal is to find an optimal allocation of $\{\mu_i\}$ under the constraint Eq. (1) so as to minimize the prevalence ρ, that is, the fraction of infected nodes.

III. THE MAXIMIZED EPIDEMIC THRESHOLD

In quenched mean-field (QMF) theory, the probability $\rho_i(t)$ that node i is infected at time t is described by N-intertwined equations [26–28],

$$\frac{d\rho_i(t)}{dt} = -\mu_i \rho_i(t) + \beta[1 - \rho_i(t)] \sum_j A_{ij}\rho_j(t). \tag{2}$$

In the steady state, $d\rho_i(t)/dt = 0$, ρ_i is determined by a set of nonlinear equations,

$$\rho_i = \frac{\beta \sum_j A_{ij}\rho_j}{\mu_i + \beta \sum_j A_{ij}\rho_j}. \tag{3}$$

One can notice that $\rho_i = 0$ is always a solution of Eq. (2). This trivial solution corresponds to an absorbing state with no infective nodes. A nonzero solution $\rho_i > 0$ exists if the effective infection rate $\lambda = \beta/\mu$ is larger than the so-called epidemic threshold λ_c. In this case, the prevalence $\rho = \sum_i \rho_i/N$ is nonzero corresponding to an endemic state. By linear stability analysis for Eq. (2) around $\rho_i = 0$, λ_c is determined by the largest eigenvalue of the matrix, $-\mathbb{U} + \beta\mathbb{A}$, which is zero, where $\mathbb{U} = \mathrm{diag}(\mu_i)$ is a diagonal matrix. For the standard SIS model, $\mu_i \equiv \mu$ for all i, one can immediately obtain the well-known result $\lambda_{c,\mathrm{QMF}}^{\mathrm{sta}} = 1/\Lambda_{\max}(\mathbb{A})$ with the largest eigenvalue of the adjacency matrix $\Lambda_{\max}(\mathbb{A})$. In our SIS model, the outbreak of epidemics will be suppressed to the greatest extent, which implies that the epidemic threshold of the optimal SIS model will be maximized.

For this purpose, we first decompose the diagonal matrix $\mathbb{U}$ into two diagonal matrices, $\mathbb{U} = \bar{U} + \Delta\mathbb{U}$, where $\bar{U} = \mathrm{diag}\{\mu k_i/\langle k\rangle\}$, with k_i being the degree of node i, and $\Delta\mathbb{U} = \mathrm{diag}\{\Delta\mu_i\}$. Since $\mathrm{Tr}(\mathbb{U}) = \mathrm{Tr}(\bar{U}) = N\mu$, $\Delta\mathbb{U}$ must satisfy the constraint $\mathrm{Tr}(\Delta\mathbb{U}) = 0$. For the real symmetric matrix, $\mathbb{U} - \beta\mathbb{A}$, its largest eigenvalue $\Lambda_{\max}$ satisfies the following inequality:

$$\Lambda_{\max} \geqslant \mathbf{v}^T(-\mathbb{U} + \beta\mathbb{A})\mathbf{v}, \tag{4}$$

where $\mathbf{v}$ is a column vector satisfying $\mathbf{v} \in \mathbb{R}^N$ and $||\mathbf{v}|| = 1$. If we set $\mathbf{v} = \frac{1}{\sqrt{N}}(1, \ldots, 1)^T$, Eq. (4) becomes

$$\Lambda_{\max} \geqslant \mathbf{v}^T(-\bar{U} + \beta\mathbb{A})\mathbf{v} - \mathbf{v}^T\Delta\mathbb{U}\mathbf{v} = -\mu + \beta\langle k\rangle. \tag{5}$$

Since $\Lambda_{\max} = 0$ at the epidemic threshold, Eq. (5) leads to an upper bound of the epidemic threshold, $\lambda_c \leqslant 1/\langle k\rangle$. The condition in which the epidemic threshold is equal to the upper bound holds when $\mathbf{v}$ is the eigenvector of $\mathbb{U} - \beta\mathbb{A}$ corresponding to its largest eigenvalue. If we set $\mathbb{U} = \bar{U}$ and $\beta = \mu/\langle k\rangle$, $-\mathbb{U} + \beta\mathbb{A} = -\mu/\langle k\rangle\mathbb{L}$, where $\mathbb{L}$ is the Laplacian matrix of the underlying network. It is well known that the smallest eigenvalue of $\mathbb{L}$ is zero and the corresponding eigenvector is $\mathbf{v}$. Therefore, if the curing rate of each node is directly proportional to its degree, i.e.,

$$\mu_i = \mu_i^* = \mu\frac{k_i}{\langle k\rangle}, \tag{6}$$

the epidemic threshold will be maximized,

$$\lambda_{c,\mathrm{QMF}}^{\mathrm{opt}} = \frac{1}{\langle k\rangle}. \tag{7}$$

In the QMF theory, the epidemic threshold of the optimal SIS model is no less than that of the standard SIS model, $\lambda_{c,\mathrm{QMF}}^{\mathrm{opt}} \geqslant \lambda_{c,\mathrm{QMF}}^{\mathrm{sta}}$, as the lower bound of $\Lambda_{\max}(\mathbb{A})$ is $\langle k\rangle$ for any types of networks [29].

The above results can also be derived from the heterogeneous mean-field (HMF) theory. In the framework of HMF, these nodes with the same degree are considered to be statistically equivalent. The constraint Eq. (1) becomes

$$\langle \mu_k \rangle = \sum\nolimits_k P(k)\mu_k = \mu \quad \text{and} \quad \mu_k \geqslant 0, \ \forall\, k, \tag{8}$$

where μ_k is the curing rate of nodes of degree k, and $P(k)$ is the degree distribution. The dynamical evolution of $\rho_k(t)$, the probability of nodes of degree k being infected at time t, reads [30]

$$\frac{d\rho_k(t)}{dt} = -\mu_k\rho_k(t) + \beta[1 - \rho_k(t)]k\Theta(t), \tag{9}$$

where Θ is the probability of finding an infected node following a randomly chosen edge. In the case of uncorrelated networks, $\Theta(t)$ can be written as

$$\Theta(t) = \sum_k \frac{kP(k)}{\langle k\rangle}\rho_k(t). \tag{10}$$

In the steady state, $d\rho_k(t)/dt = 0$, Eq. (9) becomes

$$\rho_k = \frac{\beta k\Theta}{\mu_k + \beta k\Theta}. \tag{11}$$

Substituting Eq. (11) into Eq. (10), we obtain a self-consistent equation of Θ,

$$\Theta = \sum_k \frac{kP(k)}{\langle k\rangle}\frac{\beta k\Theta}{\mu_k + \beta k\Theta}. \tag{12}$$

The epidemic threshold is determined by which derivation of the right-hand side of Eq. (12) with respect to Θ at $\Theta = 0$ is equal to 1, leading to

$$\beta_{c,\mathrm{HMF}} = \frac{\langle k\rangle}{\sum_k \frac{k^2P(k)}{\mu_k}}. \tag{13}$$

For a given $P(k)$, maximizing β_c is equivalent to minimizing the denominator of the right-hand side of Eq. (13). For this purpose, we employ the Lagrange multiplier method (LMM) to maximize the epidemic threshold, where the Lagrange function is written as

$$\mathcal{L} = \sum_k \frac{k^2P(k)}{\mu_k} + \tau\left(\sum_k P(k)\mu_k - \mu\right), \tag{14}$$

where τ is called the Lagrange multiplier. Taking the derivation of $\mathcal{L}$ with respect to μ_k,

$$\frac{\partial\mathcal{L}}{\partial\mu_k} = -\frac{k^2P(k)}{\mu_k^2} + \tau P(k). \tag{15}$$

Letting $\partial\mathcal{L}/\partial\mu_k = 0$, we have $\mu_k = k/\sqrt{\tau}$, and we insert the relation into Eq. (8). We arrive at an optimal allocation of $\{\mu_k\}$,

$$\mu_k = \mu_k^* = \mu\frac{k}{\langle k\rangle}, \tag{16}$$

and a maximal epidemic threshold by Eq. (13),

$$\lambda_{c,\mathrm{HMF}}^{\mathrm{opt}} = \frac{1}{\langle k\rangle}. \tag{17}$$

Interestingly, the HMF results are consistent with the QMF ones. Also, in the HMF theory, the epidemic threshold of the optimal SIS model is no less than that of the standard SIS model, $\lambda_{c,\mathrm{HMF}}^{\mathrm{opt}} \geqslant \lambda_{c,\mathrm{HMF}}^{\mathrm{sta}} = \langle k\rangle/\langle k^2\rangle$.

IV. NEAR-EPIDEMIC THRESHOLD

For λ larger than but close to λ_c^{opt}, $\lambda \gtrsim \lambda_c^{\mathrm{opt}}$, we shall combine perturbation theory with LMM to optimize the prevalence. Toward that end, we assume that for $\lambda = \lambda_c^{\mathrm{opt}} + \Delta\lambda$, $\mu_k = \mu_k^* + \Delta\mu_k$ and $\Theta = \Theta^* + \Delta\Theta$, where $\Theta^* = 1 - \frac{\mu}{\beta\langle k\rangle}$ is the solution of Eq. (12) for $\mu_k = \mu_k^*$. Expanding Eq. (12) around (μ_k^*, Θ^*) to second order, and then using the constraint $\sum_k P(k)\Delta\mu_k = 0$ and simultaneously ignoring the second-order small quantity $\Delta\Theta^2$, yields (see Appendix A for details)

$$\Delta\Theta = \frac{1}{\beta^2\langle k\rangle}\sum_k \frac{P(k)}{k}\Delta\mu_k^2. \tag{18}$$

Around (μ_k^*, Θ^*), the change $\Delta\rho$ in the prevalence $\rho = \sum_k P(k)\rho_k$ can be written as

$$\Delta\rho = -\frac{\Theta^*}{\beta}\sum_k \frac{P(k)}{k}\Delta\mu_k + (1-\Theta^*)\Delta\Theta. \tag{19}$$

Again using LMM to minimize $\Delta\rho$ under the constraints $\sum_k P(k)\Delta\mu_k = 0$ and Eq. (18), we obtain a minimal $\rho = \rho^* + \Delta\rho^{\mathrm{opt}}$, where $\rho^* = \sum_k P(k)\frac{\beta k\Theta^*}{\mu_k^* + \beta k\Theta^*} = 1 - \frac{1}{\lambda\langle k\rangle}$ is the prevalence for the SIS model with the fixed $\mu_k = \mu_k^*$, and

$$\begin{aligned}\Delta\rho^{\mathrm{opt}} &= -\frac{1}{4\lambda}\langle k\rangle^2(\langle k^{-1}\rangle - \langle k\rangle^{-1})\Delta\lambda^2 \\ &\simeq -\frac{1}{4}\langle k\rangle^3(\langle k^{-1}\rangle - \langle k\rangle^{-1})\Delta\lambda^2\end{aligned} \tag{20}$$

measures the difference in prevalence between the optimal SIS model and the SIS model with the fixed $\mu_k = \mu_k^*$. Since $\langle k^{-1}\rangle > \langle k\rangle^{-1}$ for any degree inhomogeneous networks in terms of Jensen's inequality, $\Delta\rho^{\mathrm{opt}} < 0$ and thus ρ will be reduced. The corresponding optimal allocation is given by $\mu_k = \mu_k^* + \Delta\mu_k$ with

$$\Delta\mu_k = \frac{\mu}{2}\langle k\rangle\lambda(\langle k\rangle - k)\Delta\lambda \simeq \frac{\mu}{2}(\langle k\rangle - k)\Delta\lambda. \tag{21}$$

This implies that as λ is increased from λ_c^{opt}, the curing rates of the nodes with degrees less than the average degree will be increased, while the curing rates of the nodes with degrees larger than the average degree will be decreased. The amplitude of the change will depend on the difference between the degree of the each node and the average degree, $\langle k\rangle - k$, and the distance of the effective infection rate to its critical value, $\Delta\lambda$.

V. GENERAL INFECTION REGION

For λ larger than but not close to λ_c^{opt}, $\lambda > \lambda_c^{\mathrm{opt}}$, since the nonlinear characteristic of the model, the analytical expression of the optimal allocation of $\{\mu_k\}$, and the corresponding minimal ρ is almost impossible. However, with the aid of HMF theory and LMM, the high-dimensional optimization problem can be converted to numerically solving the low-dimensional nonlinear equations (see Appendix B for details). In the general infection region, μ_k satisfies the following equation:

$$\mu_k = \begin{cases}\sqrt{\frac{\beta k\Theta}{\tau} + \frac{\kappa\beta k^2}{\tau\langle k\rangle}} - \beta k\Theta > 0, & k < k_c, \\ 0, & k \geqslant k_c,\end{cases} \tag{22}$$

where τ and κ are the Lagrange multipliers, and k_c is a threshold degree to guarantee $\mu_k > 0$ for $k < k_c$, and it will be determined later. Θ, τ, and κ are determined by the following

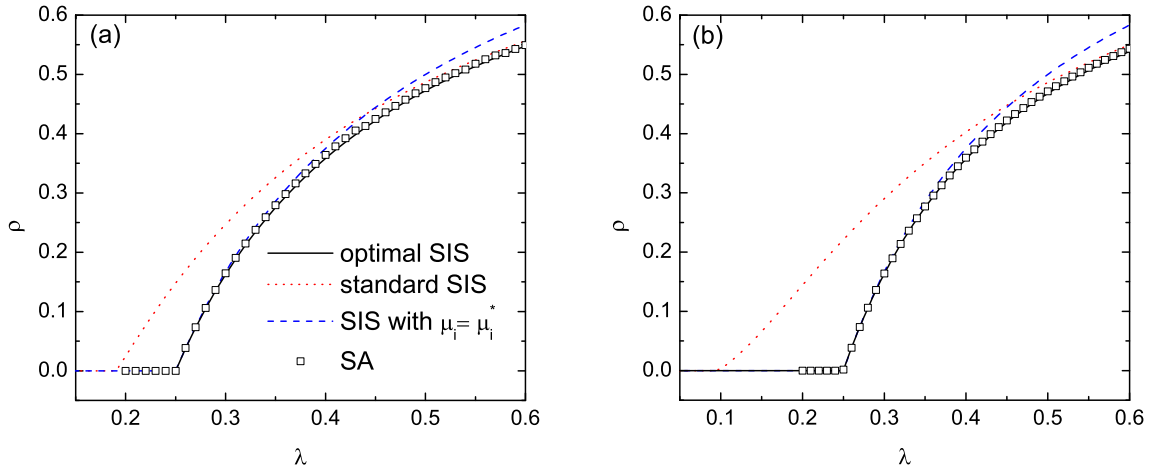

FIG. 1. Prevalence ρ vs the effective infection rate λ in ER networks (a) and BA networks (b) with equal $N = 1000$ and $\langle k \rangle = 4$. The solid lines correspond to the results from the optimal SIS model, the dotted line to the results of the standard SIS model, and the dashed line to the SIS model with $\mu_i = \mu_i^*$. The squares correspond to the results from SA.

three equations:

$$\sqrt{\frac{\beta\tau\langle k\rangle}{\Theta}}\sum_{k=k_{\min}}^{k_{\max}}\sqrt{\xi}P(k)-\beta\tau\langle k\rangle\sum_{k=k_{\min}}^{k_{\max}}\xi P(k)$$

$$-\beta\kappa\tau\sum_{k=k_{\min}}^{k_{\max}}k\xi P(k)-\frac{\kappa}{\langle k\rangle\Theta}\sum_{k=k_c}^{k_{\max}}kP(k)=0, \quad (23)$$

$$\mu=\sqrt{\frac{\beta\Theta}{\tau\langle k\rangle}}\sum_{k=k_{\min}}^{k_c}k\xi^{-\frac{1}{2}}P(k)-\beta\Theta\sum_{k=k_{\min}}^{k_c}kP(k), \quad (24)$$

$$\Theta=\sqrt{\frac{\beta\tau\Theta}{\langle k\rangle}}\sum_{k=k_{\min}}^{k_c}k^2\xi^{-\frac{1}{2}}P(k)+\frac{1}{\langle k\rangle}\sum_{k=k_c}^{k_{\max}}kP(k), \quad (25)$$

where we have used $\xi = k/(\langle k\rangle + \kappa k)$.

To numerically solve Θ, τ, and κ with Eqs. (23), (24), and (25), k_c must be known in advance. Toward that end, we adopt a numerical scheme as follows. (i) First, we set $k_c = k_{\max}$, where $k_{\max}$ is the maximal degree of the underlying network; (ii) we numerically solve Θ, τ, and κ using Eqs. (23), (24), and (25), and then we test the condition $\mu_k > 0$ for all $k < k_c$ using Eq. (22); and (iii) if the condition is not satisfied, k_c will be decreased by $k_c \leftarrow k_c - 1$ and return to (ii) until the condition Eq. (22) is fulfilled.

VI. THEORETICAL AND SIMULATION RESULTS

Figure 1 shows the optimized results of ρ as a function λ (solid line) in Erdös-Rényi (ER) random networks (a) and Barabási-Albert scale-free networks (b) with equal network size $N = 1000$ and average degree $\langle k\rangle = 4$. For comparison, we also show the results of the standard SIS model (dotted line) and of the SIS model with the curing rates $\mu_i = \mu_i^*$ (dashed line). As expected by the theoretical prediction, the epidemic threshold of the optimal SIS model $\lambda_c^{\text{opt}} = 1/\langle k\rangle$, which is significantly larger than that of the standard SIS model [obtained by numerically solving Eq. (3) for $\mu_i \equiv \mu$], but it coincides with the case of $\mu_i = \mu_i^*$. In contrast, for $\lambda > \lambda_c^{\text{opt}}$, the prevalence for $\mu_i = \mu_i^*$ is always larger than the optimal choice, and even larger than the standard SIS model in the strong infection region, indicating that $\mu_i = \mu_i^*$ is not a good choice once the epidemic outbreak has happened.

We use the simulated annealing (SA) technique [31] to validate our theoretical results. SA builds a Monte Carlo Markov chain that in the long run converges to the minimum of a given energy function $\mathcal{E}$, where $\mathcal{E} = \rho$ can be obtained by numerically iterating Eq. (3). The main steps of SA are as follows. At the beginning, we assign to a given set of $\{\mu_i\}$ satisfying the constraint Eq. (1) (e.g., $\mu_i = \mu$ for all i). Then, we randomly choose two distinct nodes, say i and j, and try to make the changes $\mu_i \leftarrow \mu_i + \delta$ and $\mu_j \leftarrow \mu_j - \delta$ with the standard METROPOLIS probability $\min(1, e^{-\beta_{\text{SA}}\Delta\mathcal{E}})$, where δ is randomly chosen between $-\mu_i$ and $\mu_i + \mu_j$ to guarantee the curing rate is always not less than zero. β_{SA} is the inverse temperature of SA, which slowly increases from 10^{-2} to 10^4 via an annealing protocol. $\Delta\mathcal{E}$ is the change of the energy function $\mathcal{E}$ due the change of μ_i and μ_j, We tested several different annealing protocols, and we adopted one in which the inverse temperature of SA, β_{SA}, is updated by $\beta_{\text{SA}} \leftarrow 1.01\beta_{\text{SA}}$ after each N attempt for updating $\{\mu_i\}$. The SA results are also shown in Fig. 1 (square dots), which agree with the theoretical prediction.

In Fig. 2, we show the optimal allocation of $\{\mu_k\}$ as a function of node degree k for several distinct λ in ER random networks (a) and BA scale-free networks (b), in which the theoretical results and the SA ones are indicated by the lines and dots, respectively. For $\lambda \gtrsim \lambda_c^{\text{opt}}$, μ_k increases linearly as k with the slope depending on the distance to the epidemic threshold. The results have been well predicted by Eqs. (16) and (21). For the region away from the threshold, μ_k will deviate from a linear relation with k. For sufficiently large λ, μ_k for large k can be less than that for small k, and even μ_k vanishes when k exceeds a threshold value, as given by Eq. (22). This surprising result implies that in the strong infection region, more medical resources should be put into these low-degree nodes rather than the high-degree nodes.

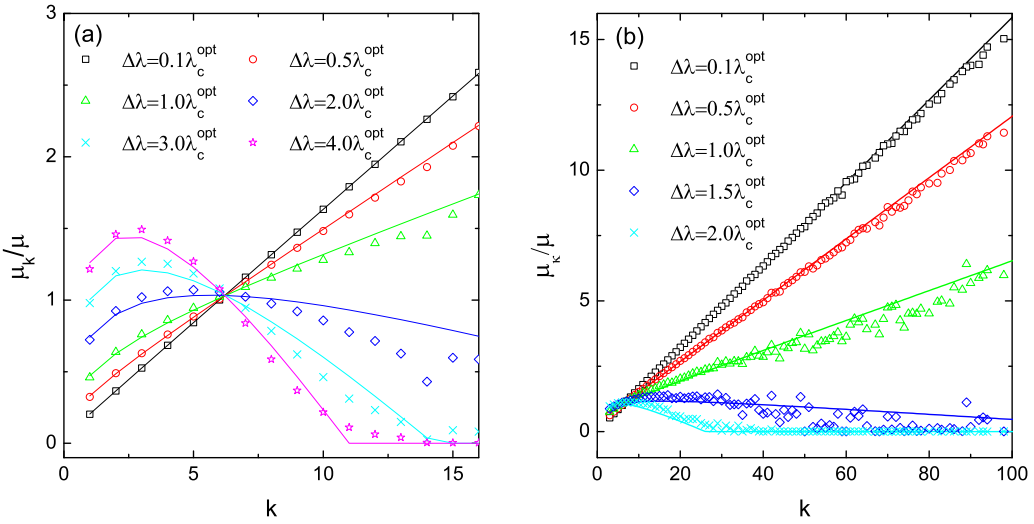

FIG. 2. The optimal allocation of $\{\mu_k\}$ as a function of node degree k for several distinct λ in ER random networks (a) and BA scale-free networks (b) with equal $N = 1000$ and $\langle k\rangle = 6$. The lines and dots indicate the theoretical and SA results, respectively.

VII. CONCLUSIONS AND PERSPECTIVE

In conclusion, we have theoretically studied the constraint optimization problem of how best to distribute limited medical resources (curing rates) to control an epidemic of SIS type. Based on the QMF and HMF theories, we have shown that the optimal allocation lies in the effective infection rate λ (or the basic reproduction number $R_0 = \langle k\rangle\lambda$). If $R_0 \leqslant 1$, the curing rate of each node should be in direct proportion to its degree under which the epidemic outbreak will be suppressed to the greatest extent and the epidemic threshold will be maximized, Eq. (7) or Eq. (17). Once the maximal epidemic threshold is just crossed ($R_0 \gtrsim 1$), the epidemic will spread persistently. In this case, we have shown analytically that the change in the curing rate of each node depends linearly on the difference between the average degree and its degree and the distance to epidemic threshold, Eq. (21). For the general infection region ($R_0 > 1$), it is almost impossible to derive an analytical solution of the optimization problem; however, it can be simplified to a much easier problem of numerical calculation of three nonlinear equations, Eqs. (23)–(25). Surprisingly, we found that in the strong infection region, the curing rates of the low-degree nodes can overpower those of the high-degree nodes to ensure minimization of prevalence.

A direct generalization for resource allocation is in the form of vaccination for prevention rather than curing, that is, the allocation is formally related to the infection rate β, not the curing rate μ. Since the prevalence is determined by the reproduction number defined by the ratio β/μ, our results maybe provide some reference value for the generalization. Another interesting generalization is how to solve the present constraint optimization problem based on other existing theoretical methods, such as the pair mean-field method, that takes into account the role of dynamical correlations between neighboring nodes [32–40]. Moreover, the method presented here could be applied to a number of other optimization problems, such as controlling opinion dynamics in social networks [41]. This will be a subject of future work.

ACKNOWLEDGMENTS

This work was supported by the National Natural Science Foundation of China (Grants No. 11205002, No. 61473001, and No. 21673212), the Key Scientific Research Fund of Anhui Provincial Education Department (Grant No. KJ2016A015), and "211" Project of Anhui University (Grant No. J01005106).

APPENDIX A: WEAK INFECTION REGION

For λ larger than but close to $\lambda_c^{\rm opt}$, $\lambda \gtrsim \lambda_c^{\rm opt}$, we have combined perturbation theory with the Lagrange multiplier method (LMM) to optimize the prevalence ρ. For $\lambda = \lambda_c^{\rm opt} + \Delta\lambda$, we have $\mu_k = \mu_k^* + \Delta\mu_k$ and $\Theta = \Theta^* + \Delta\Theta$, where $\mu_k^* = \mu k/\langle k\rangle$, and $\Theta^* = 1 - \frac{\mu}{\beta\langle k\rangle}$ is the solution of the self-consistent equation of Θ, Eq. (12) in the main text, under $\mu_k = \mu_k^*$. Since $\Theta > 0$ in the region of epidemic spreading, Eq. (12) in the main text can be rewritten as

$$\frac{\beta}{\langle k\rangle}\sum_k \frac{k^2 P(k)}{\mu_k + \beta k\Theta} = 1. \tag{A1}$$

Expanding the above equation around (μ_k^*, Θ^*) to second order yields

$$\begin{aligned}&\sum_k \frac{\partial f}{\partial \mu_k}\bigg|_{(\mu_k^*,\Theta^*)}\Delta\mu_k + \frac{\partial f}{\partial\Theta}\bigg|_{(\mu_k^*,\Theta^*)}\Delta\Theta \\ &+\frac{1}{2}\sum_k\sum_{k'}\frac{\partial^2 f}{\partial\mu_k\partial\mu_{k'}}\bigg|_{(\mu_k^*,\Theta^*)}\Delta\mu_k\Delta\mu_{k'} \\ &+\sum_k \frac{\partial^2 f}{\partial\mu_k\partial\Theta}\bigg|_{(\mu_k^*,\Theta^*)}\Delta\mu_k\Delta\Theta + \frac{1}{2}\frac{\partial^2 f}{\partial\Theta\partial\Theta}\bigg|_{(\mu_k^*,\Theta^*)}\Delta\Theta^2 = 0,\end{aligned} \tag{A2}$$

where $f \triangleq \frac{\beta}{\langle k\rangle}\sum_k \frac{k^2P(k)}{\mu_k+\beta k\Theta}-1$, and

$$\left.\frac{\partial f}{\partial \mu_k}\right|_{(\mu_k^*,\Theta^*)} = -\frac{P(k)}{\beta\langle k\rangle},$$
$$\left.\frac{\partial f}{\partial \Theta}\right|_{(\mu_k^*,\Theta^*)} = -1,$$
$$\left.\frac{\partial^2 f}{\partial \mu_k \partial \mu_{k'}}\right|_{(\mu_k^*,\Theta^*)} = \delta_{kk'}\frac{2P(k)}{\beta^2\langle k\rangle k},$$
$$\left.\frac{\partial^2 f}{\partial \mu_k \partial \Theta}\right|_{(\mu_k^*,\Theta^*)} = \frac{2P(k)}{\beta\langle k\rangle},$$
$$\left.\frac{\partial^2 f}{\partial \Theta \partial \Theta}\right|_{(\mu_k^*,\Theta^*)} = 2. \tag{A3}$$

Substituting Eq. (A3) into Eq. (A2), we obtain

$$-\frac{1}{\beta\langle k\rangle}\sum_k P(k)\Delta\mu_k - \Delta\Theta + \frac{1}{\beta^2\langle k\rangle}\sum_k \frac{P(k)}{k}\Delta\mu_k^2 + \frac{2}{\beta\langle k\rangle}\sum_k P(k)\Delta\mu_k\Delta\Theta + \Delta\Theta^2 = 0. \tag{A4}$$

Using the constraint $\sum_k P(k)\Delta\mu_k = 0$ and ignoring the second-order small quantity $\Delta\Theta^2 \ll \Delta\Theta$, Eq. (A4) becomes

$$\Delta\Theta = \frac{1}{\beta^2\langle k\rangle}\sum_k \frac{P(k)}{k}\Delta\mu_k^2. \tag{A5}$$

Around (μ_k^*,Θ^*), the change $\Delta\rho$ in the prevalence $\rho = \sum_k P(k)\rho_k$ can be expanded in leading order,

$$\Delta\rho = \sum_k \left.\frac{\partial\rho}{\partial\mu_k}\right|_{(\mu_k^*,\Theta^*)}\Delta\mu_k + \left.\frac{\partial\rho}{\partial\Theta}\right|_{(\mu_k^*,\Theta^*)}\Delta\Theta, \tag{A6}$$

where

$$\left.\frac{\partial\rho}{\partial\mu_k}\right|_{(\mu_k^*,\Theta^*)} = -\frac{P(k)\Theta^*}{\beta k},$$
$$\left.\frac{\partial\rho}{\partial\Theta}\right|_{(\mu_k^*,\Theta^*)} = 1-\Theta^*. \tag{A7}$$

Substituting Eq. (A7) into Eq. (A6), we obtain

$$\Delta\rho = -\frac{\Theta^*}{\beta}\sum_k \frac{P(k)}{k}\Delta\mu_k + (1-\Theta^*)\Delta\Theta. \tag{A8}$$

In the following, we use LMM to minimize $\Delta\rho$ under the constraints $\sum_k P(k)\Delta\mu_k = 0$ and Eq. (A5). Note that the first constraint is due to the fixed average curing rate, and the second one is the requirement of the HMF dynamics. Utilizing Eq. (A8) and the two constraints, the Lagrange function can be written as

$$\mathcal{L} = -\frac{\Theta^*}{\beta}\sum_k \frac{P(k)}{k}\Delta\mu_k + (1-\Theta^*)\Delta\Theta + \tau\left(-\Delta\Theta + \frac{1}{\beta^2\langle k\rangle}\sum_k \frac{P(k)}{k}\Delta\mu_k^2\right) + \kappa\sum_k P(k)\Delta\mu_k, \tag{A9}$$

where τ and κ are the Lagrange multipliers. Taking the derivative of $\mathcal{L}$ with respect to $\Delta\Theta$ and $\Delta\mu_k$, we obtain

$$\frac{\partial\mathcal{L}}{\partial\Delta\Theta} = (1-\Theta^*) - \tau \tag{A10}$$

and

$$\frac{\partial\mathcal{L}}{\partial\Delta\mu_k} = -\frac{\Theta^*}{\beta}\frac{P(k)}{k} + \tau\frac{1}{\beta^2\langle k\rangle}\frac{2P(k)}{k}\Delta\mu_k + \kappa P(k). \tag{A11}$$

Letting $\frac{\partial L}{\partial\Delta\Theta} = 0$ and $\frac{\partial L}{\partial\Delta\mu_k} = 0$, we obtain

$$\tau = 1-\Theta^* \tag{A12}$$

and

$$-\frac{\Theta^*}{\beta k} + \frac{2\tau}{\beta^2 k\langle k\rangle}\Delta\mu_k + \kappa = 0, \tag{A13}$$

respectively. Substituting Eq. (A13) into the constraint $\sum_k P(k)\Delta\mu_k = 0$, we obtain

$$\kappa = \frac{\Theta^*}{\beta\langle k\rangle}. \tag{A14}$$

Combining Eqs. (A12), (A13), and (A14), we obtain

$$\Delta\mu_k = \frac{\mu}{2}\langle k\rangle\lambda(\langle k\rangle - k)\Delta\lambda \simeq \frac{\mu}{2}(\langle k\rangle - k)\Delta\lambda. \tag{A15}$$

Substituting Eq. (A5) and Eq. (A15) into Eq. (A8), we obtain

$$\Delta\rho^{\text{opt}} = -\frac{1}{4\lambda}\langle k\rangle^2\left(\langle k^{-1}\rangle - \langle k\rangle^{-1}\right)\Delta\lambda^2 \simeq -\frac{1}{4}\langle k\rangle^3\left(\langle k^{-1}\rangle - \langle k\rangle^{-1}\right)\Delta\lambda^2. \tag{A16}$$

APPENDIX B: GENERAL INFECTION REGION

For λ larger than but not close to λ_c^{opt}, due to the nonlinear character of the model, an analytical expression of the optimal allocation of $\{\mu_k\}$ and the corresponding minimal ρ is in general impossible. However, with the aid of HMF theory and LMM, the high-dimensional optimization problem can be converted to numerically solving low-dimensional nonlinear equations. We first write a Lagrange function as

$$\mathcal{L} = \sum_k P(k)\frac{\beta k\Theta}{\mu_k+\beta k\Theta} + \tau\left(\sum_k P(k)\mu_k - \mu\right) + \kappa\left(\sum_k \frac{kP(k)}{\langle k\rangle}\frac{\beta k\Theta}{\mu_k+\beta k\Theta} - \Theta\right), \tag{B1}$$

where τ and κ are the Lagrange multipliers. Taking the derivative of $\mathcal{L}$ with respect to μ_k and Θ, we obtain

$$\frac{\partial \mathcal{L}}{\partial \mu_k} = -P(k)\frac{\beta k\Theta}{(\mu_k+\beta k\Theta)^2} + \tau P(k) - \kappa \frac{kP(k)}{\langle k\rangle}\frac{\beta k\Theta}{(\mu_k+\beta k)^2} \tag{B2}$$

and

$$\frac{\partial \mathcal{L}}{\partial \Theta} = \sum_k \frac{\beta k P(k)}{\mu_k+\beta k\Theta} - \sum_k \frac{\beta^2 k^2 P(k)\Theta}{(\mu_k+\beta k\Theta)^2} - \kappa \sum_k \frac{kP(k)}{\langle k\rangle}\frac{\beta^2 k^2\Theta}{(\mu_k+\beta k\Theta)^2}. \tag{B3}$$

Taking the derivative of $\mathcal{L}$ with respect to the Lagrange multipliers τ and κ, we obtain the constraint equation (8) and the self-consistent equation (12) of Θ in the main text.

Letting $\partial\mathcal{L}/\partial\mu_k = 0$, we obtain

$$\mu_k = \begin{cases} \sqrt{\frac{\beta k\Theta}{\tau} + \frac{\kappa\beta k^2}{\tau\langle k\rangle}} - \beta k\Theta > 0, & k < k_c, \\ 0, & k \geqslant k_c, \end{cases} \tag{B4}$$

where k_c is a threshold degree to guarantee $\mu_k > 0$ for $k < k_c$, and it will be determined later. Substituting Eq. (B4) into Eq. (B3) and letting $\partial\mathcal{L}/\partial\Theta = 0$, we obtain

$$\sqrt{\frac{\beta\tau\langle k\rangle}{\Theta}}\sum_{k=k_{\min}}^{k_c}\frac{P(k)\sqrt{k}}{\sqrt{\langle k\rangle+\kappa k}} - \beta\tau\langle k\rangle\sum_{k=k_{\min}}^{k_c}\frac{P(k)k}{\langle k\rangle+\kappa k} - \beta\kappa\tau\sum_{k=k_{\min}}^{k_c}\frac{P(k)k^2}{\langle k\rangle+\kappa k} - \frac{\kappa}{\langle k\rangle\Theta}\sum_{k=k_c}^{k_{\max}} kP(k) = 0. \tag{B5}$$

Combining Eq. (8) in the main text and Eq. (B4), we obtain

$$\mu = \sqrt{\frac{\beta\Theta}{\tau\langle k\rangle}}\sum_{k=k_{\min}}^{k_c} P(k)\sqrt{k}\left(\sqrt{\langle k\rangle+\kappa k}\right) - \beta\Theta\sum_{k=k_{min}}^{k_c} P(k)k. \tag{B6}$$

Combining Eq. (12) in the main text and Eq. (B4), we obtain

$$\Theta = \sqrt{\frac{\beta\tau\Theta}{\langle k\rangle}}\sum_{k=k_{\min}}^{k_c}\frac{P(k)k^{3/2}}{\sqrt{\langle k\rangle+\kappa k}} + \frac{1}{\langle k\rangle}\sum_{k=k_c}^{k_{\max}} kP(k). \tag{B7}$$

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