

ESTIMATION OF CONTROL ENERGY AND CONTROL STRATEGIES FOR COMPLEX NETWORKS

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The controlling of complex networks is one of the most challenging problems in modern network science. Accordingly, the required energy cost of control is a fundamental and significant problem. In this paper, we present the theoretical analysis and numerical simulations to study the controllability of complex networks from the energy perspective. First, by combining theoretical derivation and numerical simulations, we obtain lower bounds of the maximal and minimal energy costs for an arbitrary normal network, which are related to the eigenvalues of the state transition matrix. Second, we deduce that controlling unstable normal networks is easier than controlling stable normal networks with the same size. Third, we demonstrate a tradeoff between the control energy and the average degree (or the maximum degree) of an arbitrary undirected network. Fourth, numerical simulations show that the energy cost is negatively correlated with the degree of nodes. Moreover, the combinations of control nodes with the greater sum of degree need less energy to implement complete control. Finally, we propose a multi-objective

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optimization model to obtain the control strategy, which not only ensures the fewer control nodes but also guarantees the less energy cost of control.

Keywords: Complex networks; controllability; control energy; control strategy; multi-objective optimization.

1. Introduction

In many areas of science and engineering, a number of realistic systems can be represented as complex networks, such as telecommunication networks, computer networks, biological networks, cognitive and semantic networks, and social networks [2, 8, 22, 17, 12, 13]. The controllability of complex networks becoming one of the most important and challenging problems in these fields. In recent years, many progresses have been made in the study of controllability of complex networks [15, 25, 34, 7, 31, 4, 23, 30]. However, even if a network is controllable in principle, it may not be controllable in practice if it costs an infinite amount of energy or if it requires too much time to achieve the control goal [33]. Therefore, the energy cost of control is an important and unavoidable problem when controlling a complex network in practice.

To identify a degree of quality of complete controllability, Muller *et al.* proposed three energy-related measures: trace, determinant and maximum eigenvalue of the inverse characteristic Gramian matrix [21]. Based on these three measures, Yan *et al.* showed reasonable bounds for estimating the lower and upper control energies [33]. Pasqualetti *et al.* focused on the tradeoffs between control energy and the number of control nodes, and on the design of a distributed control strategy, as opposed to scaling laws for the control energy as a function of the control horizon [24]. Summers and Lygeros showed an important class of metrics based on the controllability and observability Gramians [27]. Sun and Motter revealed that there is a tradeoff between nonlocality of the control trajectory in the phase space and nonlocality of the control inputs in the network itself [28]. More recent study demonstrated that several classes of energy-related controllability metrics have a strong structural property, which is called submodularity [5].

Despite great advances in the quantitative evaluation of controllability of complex networks, there are still many problems that are deserved to be explored, for example, the relationship between network topology and its energy cost of control, and setting up the control strategy not only ensures the fewer control nodes but also guarantees the lower energy cost for controlling complex networks.

In this study, we focus on estimating the bounds of energy cost for controlling complex networks by using the matrix algebra theory and graph theory, especially quantifying the minimal energy cost E_{\min} and the maximal energy cost E_{\max} , respectively. By combining theoretical derivation and numerical simulations, we reveal how the network structure and node degree may affect the energy cost. Based on these preliminary results, we propose a multi-objective optimization model to

design control strategy of complex networks, which not only ensures the fewer control nodes but also guarantees the lower energy cost of controllability. These results provide an important step on controllability towards ultimately realistic control of complex networks.

2. The Dynamical Description of Complex Networks and Preliminary Results

To explore the energy cost of complex networks, we study the linear time-invariant dynamic system [16]. Suppose that the network dynamics with n nodes can be described by the following time-invariant ordinary differential equations (ODEs)

$$\frac{dx(t)}{dt} = Ax(t) + Bu(t), \tag{1}$$

where $x(t) = (x_1(t), \dots, x_n(t))^T$ stands for states of n nodes at time t , for example, $x_i(t)$ can be the concentration of mRNAs in a gene regulatory network. Matrix $A \in R^{n \times n}$ stands for the state transition matrix of the system, describing system interactions strength of links, a_{ij} represents the weight of a directed link from node j to i . Matrix $B \in R^{n \times m}$ stands for the control matrix, $u(t) = (u_1(t), \dots, u_m(t))^T$ stands for the m control signals.

The network described by Eq. (1) is said to be completely controllable if it can be steered from any initial state to any desired final state in finite time. The Kalman controllability matrix of a network can be defined as follows:

$$C = [B, AB, \dots, A^{n-1}B]. \tag{2}$$

The network is completely controllable if and only if the Kalman controllability matrix has full rank [11], that is

$$\text{rank}(C) = n. \tag{3}$$

To be able to apply Eq. (3) to an arbitrary network, we need to know the values of elements in matrices A and B . However, for most real complex networks, they are either unknown or are known only approximately and are time dependent. Lin [14] proposes a concept of structural controllability. Controllability of complex networks is addressed in terms of structural control theory [15], where a maximum matching algorithm in graph theory is used to identify the minimal set of driver nodes to control an entire network.

For the n -dimensional linear time-invariant dynamics, giving the certain initial state $x_0 = 0$, the certain target state x_f and the time interval $[0, t_f]$, the energy cost with the control input $u(t)$ can be defined as

$$\varepsilon(u(t), t_f) = \int_0^{t_f} \|u(t)\|^2 dt. \tag{4}$$

A method to evaluate the qualities of controllability is to consider the fixed-time minimum-energy control problem. It is defined as follows [10]:

$$\begin{aligned} & \min_{u(t) \in L_2} \int_0^{t_f} \|u(t)\|^2 dt \\ & \text{s.t. } \begin{cases} \dot{x}(t) = Ax(t) + Bu(t) \\ x(0) = 0, \quad x(t_f) = x_f, [0, t_f] \text{fixed.} \end{cases} \end{aligned} \tag{5}$$

If the system is completely controllable, then the minimum control energy is given by

$$\int_0^{t_f} \|u^*(t)\|^2 dt = x_f^T W_{t_f}^{-1} x_f, \tag{6}$$

where the matrix $W_{t_f} = \int_0^{t_f} e^{At} B B^T e^{A^T t} dt$ is called the controllability Gramian matrix at time t_f , and the optimal input has the form

$$u^*(t) = B^T e^{A^T(t_f-t)} W_{t_f}^{-1} x_f. \tag{7}$$

For the Gramian matrix, it is positive definite when the system is completely controllable. In the following, we focus on the normalized energy cost [33]:

$$E(u(t), t_f) = \varepsilon(u(t), t_f) / \|x_f\|^2 = \frac{x_f^T W_{t_f}^{-1} x_f}{x_f^T x_f}. \tag{8}$$

Based on the Rayleigh–Ritz theorem [6], the bound of the normalized energy cost [33] was given by

$$\frac{1}{\lambda_{\max}(W_{t_f})} = E_{\min} \leq E(u(t), t_f) \leq E_{\max} = \frac{1}{\lambda_{\min}(W_{t_f})}, \tag{9}$$

where $\lambda_{\max}(W_{t_f})$ and $\lambda_{\min}(W_{t_f})$ are the maximal and minimal eigenvalues of the controllability Gramian matrix W_{t_f} , respectively, and E_{\min} and E_{\max} are called the minimal energy and the maximal energy, respectively.

In the following, we use two energy-related measures of controllability, i.e., trace and maximum eigenvalue of the inverse characteristic Gramian matrix [33]. The first measure of controllability is given by the average value of the minimum control energy over the unit hypersphere $\{x : \|x\| = 1\}$. For practical applications, it is desirable to maintain the average costs in Eq. (10) as small as possible

$$\frac{\int_{\|x\|=1} x^T W_{t_f}^{-1} x dx}{\int_{\|x\|=1} dx} = \frac{1}{n} \text{tr} W_{t_f}^{-1}. \tag{10}$$

Another measure of controllability is given by the maximum value of the minimum control energy over the unit ball $\{x : \|x\| = 1\}$ as shown in Eq. (11). For real systems it is desirable to have the maximum eigenvalue of $W_{t_f}^{-1}$ as small as possible

$$\max_{\|x\|=1} x^T W_{t_f}^{-1} x = \lambda_{\max}(W_{t_f}^{-1}) = \frac{1}{\lambda_{\min}(W_{t_f})}. \tag{11}$$

3. Bounds of Control Energy for Complex Networks

3.1. Lower bounds of maximal and minimal energy costs

Theorem 3.1. Consider a network $G = (V, E)$ with $|V| = n$, weighted adjacency matrix A , and control set K . For any certain initial state x_0 and any certain target state x_f , if the system can transform between x_0 and x_f in the finite time $[0, t_f]$. Assume that $\lambda_{\min}(A+A^T) \neq 0$ and A is a normal matrix, then it holds

$$E_{\max} \geq \frac{\lambda_{\min}(A+A^T)}{e^{t_f \lambda_{\min}(A+A^T)} - 1}, \tag{12}$$

$$E_{\min} \geq \frac{\lambda_{\max}(A+A^T)}{e^{t_f \lambda_{\max}(A+A^T)} - 1}. \tag{13}$$

Proof. Because

$$\begin{aligned} W_{t_f}^{(n)} &= \int_0^{t_f} \Phi(t_f, s) B B^T \Phi^T(t_f, s) ds \\ &= \int_0^{t_f} \Phi(t_f, s) \Phi^T(t_f, s) ds = \int_0^{t_f} e^{(t_f-s)(A+A^T)} ds \\ &= \int_0^{t_f} \sum_{n=0}^{\infty} \frac{(t_f-s)^n (A+A^T)^n}{n!} ds = \sum_{n=0}^{\infty} \frac{(A+A^T)^n}{n!} \int_0^{t_f} (t_f-s)^n ds \\ &= \sum_{n=0}^{\infty} \frac{(A+A^T)^n t_f^{n+1}}{n! (n+1)}. \end{aligned}$$

Then

$$\begin{aligned} &\lambda_{\min}(W_{t_f}^{(K)}) \\ &\leq \lambda_{\min}(W_{t_f}^{(n)}) = \lambda_{\min} \left(\sum_{n=0}^{\infty} \frac{(A+A^T)^n t_f^{n+1}}{n! (n+1)} \right) \\ &= \sum_{n=0}^{\infty} \frac{(\lambda_{\min}(A+A^T))^n t_f^{n+1}}{n! (n+1)} \\ &= \frac{1}{\lambda_{\min}(A+A^T)} \sum_{n=0}^{\infty} \frac{(\lambda_{\min}(A+A^T) t_f)^{n+1}}{(n+1)!} \\ &= \frac{e^{t_f \lambda_{\min}(A+A^T)} - 1}{\lambda_{\min}(A+A^T)}. \end{aligned}$$

Therefore

$$E_{\max} = \frac{1}{\lambda_{\min}(W_{t_f}^{(K)})} \geq \frac{\lambda_{\min}(A+A^T)}{e^{t_f \lambda_{\min}(A+A^T)} - 1}.$$

In a similar way, we can also prove

$$E_{\min} \geq \frac{\lambda_{\max}(A+A^T)}{e^{t_f \lambda_{\max}(A+A^T)} - 1}.$$

For convenience in following discussion, we denote that

$$E_{\max-LB} = \frac{\lambda_{\min}(A+A^T)}{e^{t_f \lambda_{\min}(A+A^T)} - 1} \quad E_{\min-LB} = \frac{\lambda_{\max}(A+A^T)}{e^{t_f \lambda_{\max}(A+A^T)} - 1}. \quad (14)$$

□

Corollary 3.1. Consider a network $G = (V, E)$ with $|V| = n$, weighted adjacency matrix $A(A = A^T)$, and control set K . For any certain initial state x_0 and any certain target state x_f , assume that the system can transform between x_0 and x_f in the finite time $[0, t_f]$, and $\lambda_{\min}(A) \neq 0$, then it holds

$$E_{\max} \geq \frac{2\lambda_{\min}(A)}{e^{2t_f \lambda_{\min}(A)} - 1}, \quad (15)$$

$$E_{\min} \geq \frac{2\lambda_{\max}(A)}{e^{2t_f \lambda_{\max}(A)} - 1}. \quad (16)$$

3.2. Numerical simulations of bounds

To validate the estimated bounds in Theorem 3.1, we simulate one simple network and two random networks with 100 nodes, i.e., ER [3] and BA networks [1]. As shown in Fig. 1(a), this simple normal network is composed of 3 nodes and 6 edges, where A is the adjacency matrix and an input control signal directly to control the node 1. In two random networks, A is the adjacency matrix, in which

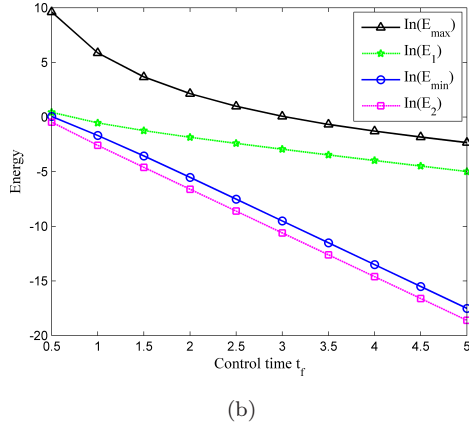
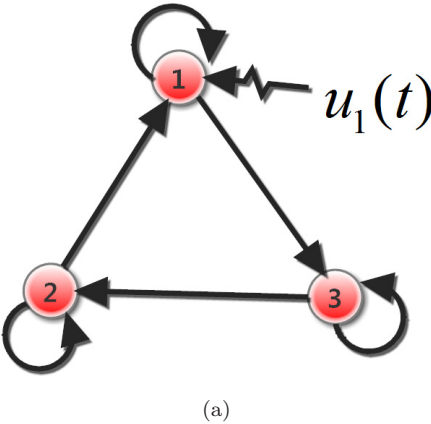


Fig. 1. (a) A simple normal network diagram, which is composed of 3 nodes and 6 edges. In this network, A is the adjacency matrix and an input control signal directly to control the node 1. (b) The curves of the energy costs evolve over time t_f , where E_{\max} and E_{\min} represent the maximal and minimal energy costs, respectively. $E_{\max-LB}$ and $E_{\min-LB}$ represent the lower bounds of the maximal and minimal energy costs, respectively. (a) A simple normal network and (b) the numerical results of control energy.

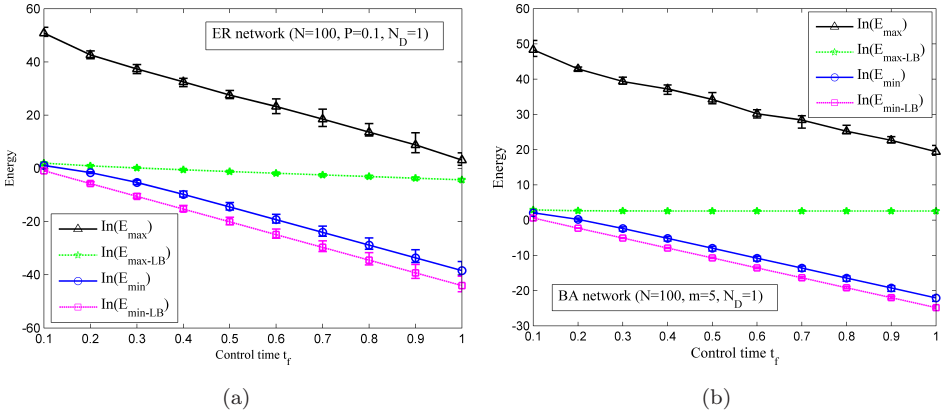


Fig. 2. The curves of the energy costs evolve with control time t_f . Here A is the adjacency matrix in which we add self-loops as $A_{ii} = \sum_{i,j=1}^n A_{ij}$, and $B = [1, 0, \dots, 0]^T$. (a) is ER network and (b) is BA network.

we add self-loops as $A_{ii} = \sum_{i,j=1}^n A_{ij}$. Using the method proposed in [15], we can find that the network is controllable by any single driver node. Therefore, we inject an input control signal on node 1. We calculate E_{\max} , E_{\min} , $E_{\max-LB}$ and $E_{\min-LB}$ according to Eqs. (9) and (14), respectively. Figures 1(b), 2(a) and 2(b) show that numerical results are consistent with our estimated bounds [see Eqs. (12) and (13)].

Remark 1. Theorem 3.1 gives a lower bound of the maximal and the minimal energy costs for an arbitrary normal network. (1) Through numerical simulations, we find that the bound estimate is reasonable. Moreover, this theorem uncovers that the energy cost of complex networks is relevant to the eigenvalue of the state transition matrix, and we can approximately estimate the range of energy cost by $\lambda_{\min}(A + A^T)$ and $\lambda_{\max}(A + A^T)$. (2) From what has been discussed above, we can easily obtain that $E_{\max} = E_{\max-LB}$ and $E_{\min} = E_{\min-LB}$ when all nodes are directly driven, and otherwise $E_{\max} > E_{\max-LB}$ and $E_{\min} > E_{\min-LB}$. More accurately, if x_f is the unit eigenvector of λ_{\min} of W_{t_f} , then $E(u^*(t), t_f) = E_{\max} = E_{\max-LB}$, and $E(u^*(t), t_f) = E_{\min} = E_{\min-LB}$ when x_f is the unit eigenvector of λ_{\max} of W_{t_f} . As shown in Fig. 3, we give optimal control signals and trajectories for the network in Fig. 1(a) at two different desired states (the unit eigenvectors of λ_{\min} and λ_{\max} of W_{t_f}).

3.3. Control time and bounds of energy costs

Theorem 3.2. Consider a network $G = (V, E)$ with $|V| = n$, weighted adjacency normal matrix A , and control set K . For any certain initial state x_0 and any certain target state x_f , assume that the system can transform between x_0 and x_f in the finite time t_f .

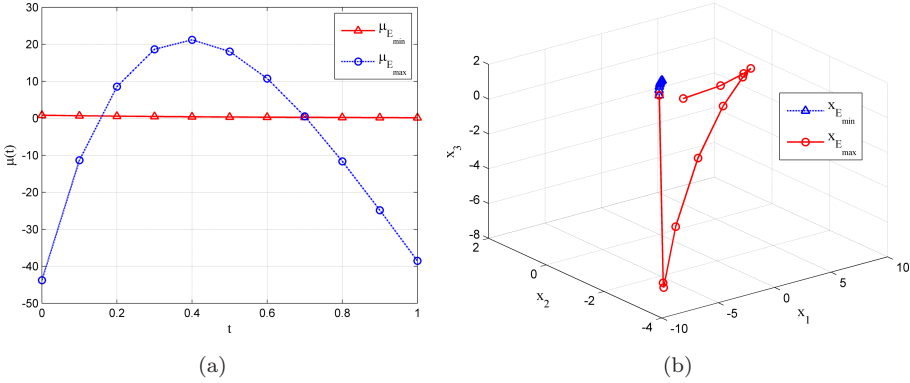


Fig. 3. (a) Optimal control signal $\mu_{E_{\min}}$ ($\mu_{E_{\max}}$) which minimizes (maximizes) the energies required to move the network from the initial state $x_0 = [0, 0, 0]^T$ to desired states $x_{E_{\min}}$ ($x_{E_{\max}}$) with $\|x_{E_{\min}}\| = 1$ ($\|x_{E_{\max}}\| = 1$) in the given time interval $t \in [0, 1]$, where $x_{E_{\min}}$ ($x_{E_{\max}}$) is the unit eigenvector of λ_{\max} (λ_{\min}) of W_{t_f} . (b) The trajectories of the network state $x(t)$ driven, respectively, by the control signals in (a).

1. For $E_{\max-LB}$, we have the following two conclusions:

(1) When t_f is small ($t_f \ll 1/|\lambda_{\min}(A + A^T)|$), then it holds

$$E_{\max-LB} \approx \frac{1}{t_f}.$$

(2) When t_f is large ($t_f \gg 1/|\lambda_{\min}(A + A^T)|$)

(i) $A + A^T$ is positive definite, then it holds

$$E_{\max-LB} = O(e^{-t_f \lambda_{\min}(A+A^T)})(t_f \rightarrow \infty).$$

(ii) $A + A^T$ is not positive definite, then it holds

$$E_{\max-LB} \approx -\lambda_{\min}(A + A^T).$$

(iii) $A + A^T$ is positive semi-definite, then it holds

$$E_{\max-LB} \approx \frac{1}{t_f}.$$

2. For $E_{\min-LB}$, we have the following two conclusions:

(1) When t_f is small ($t_f \ll 1/|\lambda_{\min}(A + A^T)|$), then it holds

$$E_{\min-LB} \approx \frac{1}{t_f}.$$

(2) When t_f is large ($t_f \gg 1/|\lambda_{\max}(A + A^T)|$)

(i) $A + A^T$ is not negative definite, then it holds

$$E_{\min-LB} = O(e^{-t_f \lambda_{\max}(A+A^T)})(t_f \rightarrow \infty).$$

(ii) $A + A^T$ is negative definite, then it holds

$$E_{\min-LB} \approx -\lambda_{\max}(A + A^T).$$

(iii) When the minimum eigenvalue of $A + A^T$ is zero, then it holds

$$E_{\min-LB} \approx \frac{1}{t_f}.$$

Proof. For $E_{\max-LB}$,

(1) Because $(t_f \ll 1/|\lambda_{\min}(A + A^T)|)$, then we can approximate estimate

$$e^{t_f \lambda_{\min}(A+A^T)} - 1 \approx t_f \lambda_{\min}(A + A^T).$$

Therefore, we have

$$E_{\max-LB} = \frac{\lambda_{\min}(A+A^T)}{e^{t_f \lambda_{\min}(A+A^T)} - 1} \approx \frac{\lambda_{\min}(A+A^T)}{t_f \lambda_{\min}(A+A^T)} = \frac{1}{t_f}.$$

(2) (i) Because $A + A^T$ is positive definite, then $\lambda_{\min}(A + A^T) > 0$. Therefore, when t_f is large ($t_f \gg 1/|\lambda_{\min}(A + A^T)|$), we have

$$\lim_{t_f \rightarrow \infty} \frac{\lambda_{\min}(A+A^T)}{e^{t_f \lambda_{\min}(A+A^T)} - 1} \Big/ e^{-t_f \lambda_{\min}(A+A^T)} = \lambda_{\min}(A+A^T).$$

Then

$$E_{\max-LB} = \frac{e^{t_f \lambda_{\min}(A+A^T)} - 1}{\lambda_{\min}(A+A^T)} = O(e^{-t_f \lambda_{\min}(A+A^T)})(t_f \rightarrow \infty).$$

(ii) Because $A + A^T$ is not positive definite, then $\lambda_{\min}(A + A^T) < 0$. When $(t_f \gg 1/|\lambda_{\min}(A + A^T)|)$, we can approximate estimate

$$e^{t_f \lambda_{\min}(A+A^T)} \approx 0.$$

Therefore, we have

$$E_{\max-LB} = \frac{\lambda_{\min}(A+A^T)}{e^{t_f \lambda_{\min}(A+A^T)} - 1} \approx -\lambda_{\min}(A+A^T).$$

(iii) Because $A + A^T$ is positive semi-definite, then $\lambda_{\min}(A + A^T) = 0$. we can be approximately estimated as

$$E_{\max-LB} \approx \lim_{\lambda_{\min}(A+A^T) \rightarrow 0} \frac{\lambda_{\min}(A+A^T)}{e^{t_f \lambda_{\min}(A+A^T)} - 1} = \frac{1}{t_f}. \quad \square$$

In a similar way, we can also prove above theorem for $E_{\min-LB}$.

In order to validate our results, we use three networks to calculate their energy bounds. Among these networks, $A_1 + A_1^T$ is negative definite as shown in Fig. 4(a), $A_2 + A_2^T$ is positive definite as shown in Fig. 5(a), and $A_3 + A_3^T$ is neither positive definite nor negative definite as shown in Fig. 6(a). Here the input control signal directly to control the node v_1 in three networks. According to Eq. (14), we can

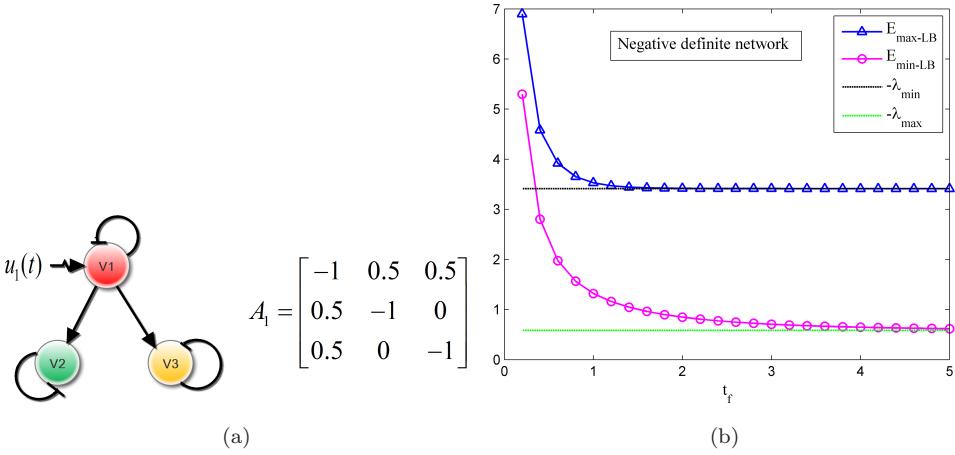


Fig. 4. This network is negative definite ($\lambda_{\min}(A_1 + A_1^T) = -3.14$ and $\lambda_{\max}(A_1 + A_1^T) = -0.59$). Here the input control signal directly to control the node v_1 . (a) The negative definite network and (b) the numerical results.

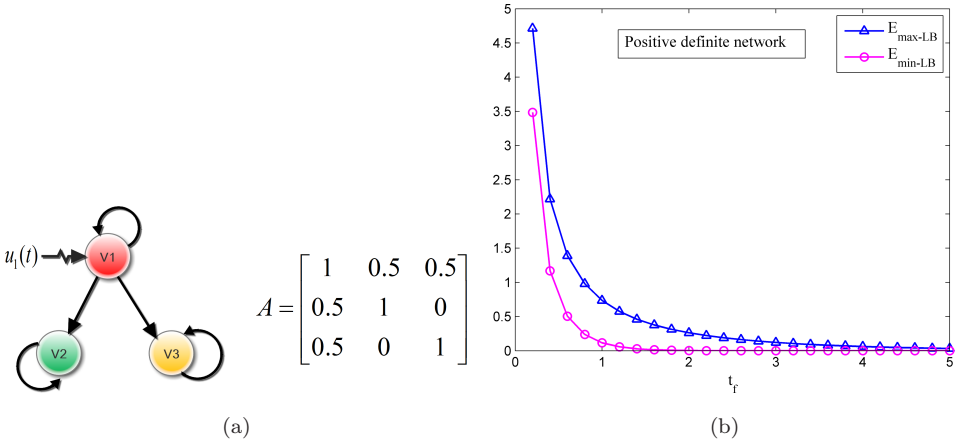


Fig. 5. This network is positive definite ($\lambda_{\min}(A_2 + A_2^T) = 0.59$ and $\lambda_{\max}(A_2 + A_2^T) = 3.14$). Here the input control signal directly to control the node v_1 . (a) The positive definite network and (b) the numerical results.

obtain the lower bounds of the maximal and the minimal energy over control time t_f . The figures at the right column in Figs. 4–6 demonstrate the correctness of the theoretical results for the estimated lower bounds of E_{\min} and E_{\max} .

Remark 2. Theorem 3.2 gives approximate estimates of lower bounds of E_{\min} and E_{\max} with the control time t_f in two different regimes separated by the characteristic time. More meaningfully, through this theorem, we discover the following results. For an arbitrary network, when it is stable, then $\lim_{t_f \rightarrow \infty} E_{\max-LB} = -\lambda_{\min}(A + A^T) > 0$ and $\lim_{t_f \rightarrow \infty} E_{\min-LB} = -\lambda_{\max}(A + A^T) > 0$. Yet, if it

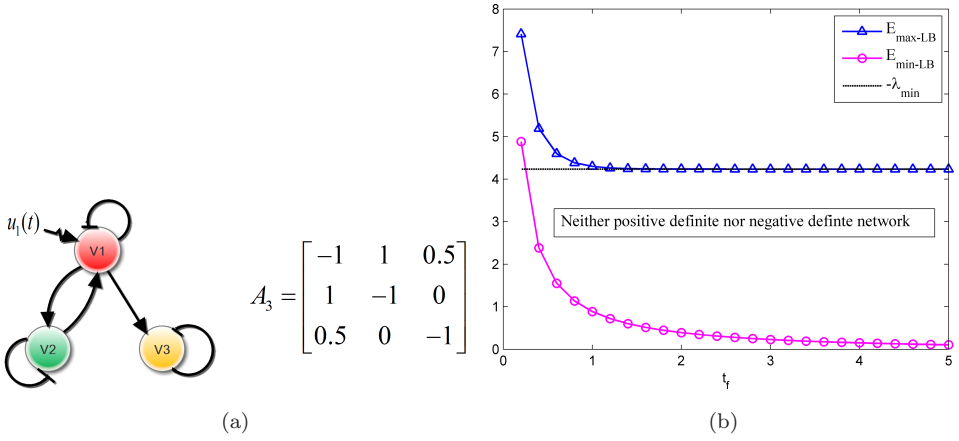


Fig. 6. (a) This network is neither positive definite nor negative definite ($\lambda_{\min}(A_3 + A_3^T) = -4.24$ and $\lambda_{\max}(A_3 + A_3^T) = 0.24$). Here the input control signal directly to control the node v_1 . (b) The numerical results of control energy.

is positive definite, then $\lim_{t_f \rightarrow \infty} E_{\max-LB} = \lim_{t_f \rightarrow \infty} E_{\min-LB} = 0$. According to Eq. (12) and (13), we find that $E_{\min} \geq -\lambda_{\max}(A + A^T) > 0$ and $E_{\max} \geq -\lambda_{\min}(A + A^T) > 0$ when it is stable, but if it is positive definite, it may be $E_{\max}, E_{\min} \rightarrow 0(t_f \rightarrow \infty)$. Therefore, we can obtain the following conclusion: controlling unstable normal networks is easier than controlling stable normal networks with the same size. In order to further validate the above claim, we simulate two simple normal networks as shown in Figs. 4(a) and 5(a) and the results are drawn in Figs. 7(a) and 7(b). These numerical results are consistent with our claim.

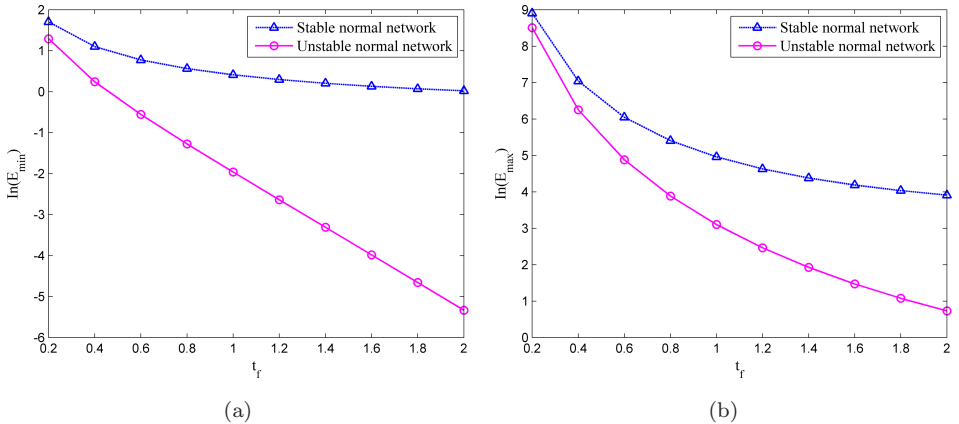


Fig. 7. (a) and (b) represent the maximal and minimal energy costs for the stable and unstable normal networks, respectively. We simulate two simple normal networks as shown in Figs. 4(a) and 5(a). Here the input control signals directly to control nodes v_1 and v_2 and (b).

4. The Degree of Nodes and Energy Cost of Control

4.1. Theoretical results

Lemma 4.1 ([32]). For an undirected graph $G = (V, E)$ with n nodes, let $A = (a_{ij})_{n \times n}$ be the adjacent matrix of G . Then the degree of vertex i is the element b_{ii} in A^2 , here $A^2 = (b_{ij})_{n \times n}$.

Lemma 4.2 ([26]). Let G be a simple connected undirected graph with n vertices, the maximum degree d_{\max} , the minimum degree d_{\min} and the spectral radius $\rho(G)$. Then

$$d_{\min} \leq \rho(G) \leq d_{\max}.$$

Lemma 4.3 ([26]). Let G be a simple connected undirected graph with n vertices, d_{\max} be the maximum degree and $d_{\text{second-max}}$ be the second largest degree. If there are p vertices with d_{\max} , then

$$\rho(G) \leq \frac{d_{\text{second-max}} - 1 + \sqrt{(d_{\text{second-max}} + 1)^2 + 4p(d_{\max} - d_{\text{second-max}})}}{2}.$$

The equality holds if and only if G is a d_{\max} -regular graph or $G \cong K_p \nabla H$, where H is a $(d_{\text{second-max}} - p)$ -regular graph with $n - p$ vertices.

Theorem 4.1. Consider a network $G = (V, E)$ with $|V| = n$, adjacency matrix $A (A = A^T)$. For any initial state x_0 and any target state x_f , assume that the system can transform between x_0 and x_f in the finite time $[0, t_f]$. Let the average degree of G be $\langle k \rangle$, when A is positive definite and t_f is big enough, we have

$$E_{\max} \geq \frac{2\sqrt{\langle k \rangle}}{e^{2t_f\sqrt{\langle k \rangle}} - 1}. \tag{17}$$

Proof. When A is positive definite, then the eigenvalues of A are $\lambda_{\max} = \lambda_n \geq \lambda_{n-1} \geq \dots \geq \lambda_1 = \lambda_{\min} > 0$. According to Lemma 4.1, we have

$$\sum_{i=1}^n k_i = \sum_{i=1}^n b_{ii} = \text{tr}(A^2) = \sum_{i=1}^n \lambda_i^2 \geq n\lambda_{\min}^2.$$

Therefore

$$\lambda_{\min} \leq \sqrt{\frac{\sum_{i=1}^n k_i}{n}} = \sqrt{\langle k \rangle}.$$

Considering a function

$$f(x) = \frac{2x}{e^{2t_f x} - 1} \quad x \in [\lambda_{\min}, \sqrt{\langle k \rangle}].$$

Taking the derivative of $f(x)$, we have

$$f'(x) = \frac{2(1 - 2t_f x)e^{2t_f x} - 2}{(e^{2t_f x} - 1)^2} \quad x \in [\lambda_{\min}, \sqrt{\langle k \rangle}].$$

When t_f is big enough, we have

$$f'(x) < 0.$$

Then

$$f(\lambda_{\min}) \geq f(\sqrt{\langle k \rangle}).$$

According to (15), we have

$$E_{\max} \geq \frac{2\lambda_{\min}(A)}{e^{2t_f\lambda_{\min}(A)} - 1} = f(\lambda_{\min}) \geq f(\sqrt{\langle k \rangle}) = \frac{2\sqrt{\langle k \rangle}}{e^{2t_f\sqrt{\langle k \rangle}} - 1}.$$

For convenience in the following discussion, we let

$$E_{\max}^{\text{degree-LB}} = \frac{2\sqrt{\langle k \rangle}}{e^{2t_f\sqrt{\langle k \rangle}} - 1}. \quad (18) \quad \square$$

Theorem 4.2. Consider a simple connected network $G = (V, E)$ with $|V| = n$, adjacency matrix $A(A = A^T)$. For any certain initial state x_0 and any certain target state x_f , assume that the system can transform between x_0 and x_f in the finite time $[0, t_f]$. Let the maximum degree of n vertices be d_{\max} and the second large degree be $d_{\text{second-max}}$. When t_f is big enough, it can be seen that

$$E_{\min} \geq \frac{2d_{\max}}{e^{2t_f d_{\max}} - 1}. \quad (19)$$

More accurately, we have

$$E_{\min} \geq \frac{2D}{e^{2t_f D} - 1}, \quad (20)$$

where $D = \frac{d_{\text{second-max}} - 1 + \sqrt{(d_{\text{second-max}} + 1)^2 + 4p(d_{\max} - d_{\text{second-max}})}}{2}$.

Proof. According to Lemma 4.2, we have

$$\lambda_{\max} = \rho(G) \leq d_{\max}.$$

Considering a function

$$f(x) = \frac{2x}{e^{2t_f x} - 1} x \in [\lambda_{\max}, d_{\max}].$$

Taking the derivative of $f(x)$, we have

$$f'(x) = \frac{2(1 - 2t_f x)e^{2t_f x} - 2}{(e^{2t_f x} - 1)^2} x \in [\lambda_{\max}, d_{\max}].$$

When t_f is big enough, we have

$$f'(x) < 0.$$

Then

$$f(\lambda_{\max}) \geq f(d_{\max}).$$

Therefore

$$E_{\min} \geq \frac{2\lambda_{\max}(A)}{e^{2t_f\lambda_{\max}(A)} - 1} = f(\lambda_{\max}) \geq f(d_{\max}) = \frac{2d_{\max}}{e^{2t_f d_{\max}} - 1}.$$

According to Lemma 4.3, we have

$$\lambda_{\max} = \rho(G) \leq D.$$

In a similar way, we can also prove

$$E_{\min} \geq \frac{2D}{e^{2t_f D} - 1}.$$

For convenience in the following discussion, we let

$$E_{\min-LB}^{\text{degree}} = \frac{2d_{\max}}{e^{2t_f d_{\max}} - 1}. \quad (21)$$

□

4.2. Numerical simulations and results analysis

According to Eqs. (18) and (21), $E_{\max-LB}^{\text{degree}}$ and $E_{\min-LB}^{\text{degree}}$ as functions of the average degree $\langle k \rangle$ (or maximum degree d_{\max}) with different values of control time t_f are shown in Figs. 8(a) and 8(b). These two figures indicate that $E_{\max-LB}^{\text{degree}}$ and $E_{\min-LB}^{\text{degree}}$ are decreasing over the average degree $\langle k \rangle$ (or maximum degree d_{\max}). Therefore, we can claim that the control energy is negatively correlated with the degree of nodes.

In order to validate our above claim, we simulate ER and BA networks and the results are drawn in Figs. 9 and 10. Here A is the adjacency matrix, in which we add self-loops as $A_{ii} = \sum_{j=1}^n A_{ij}$, and the input control signals directly to control nodes from 1 to N ($N = 1, 5, 10$ and 20) in two networks. From these figures, we

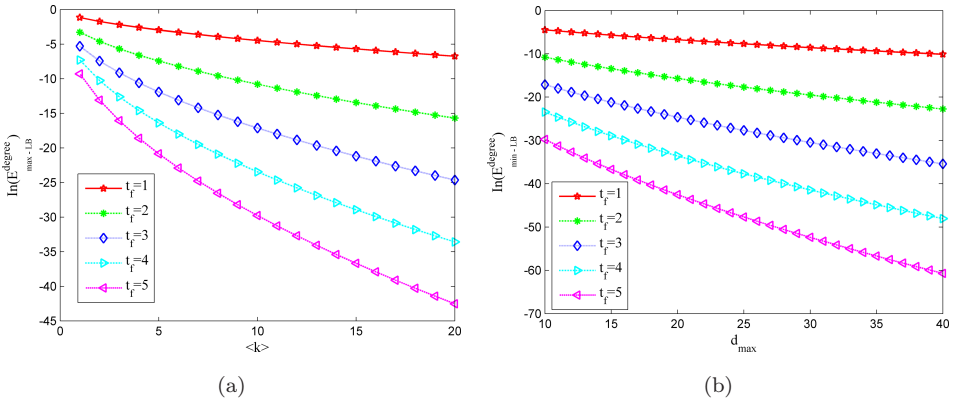


Fig. 8. These two subfigures indicate the relationship between the lower of control energy and the degree of nodes. (a) $E_{\max-LB}^{\text{degree}}$ as a function of $\langle k \rangle$ with different values of t_f and (b) $E_{\min-LB}^{\text{degree}}$ as a function of d_{\max} with different values of t_f .

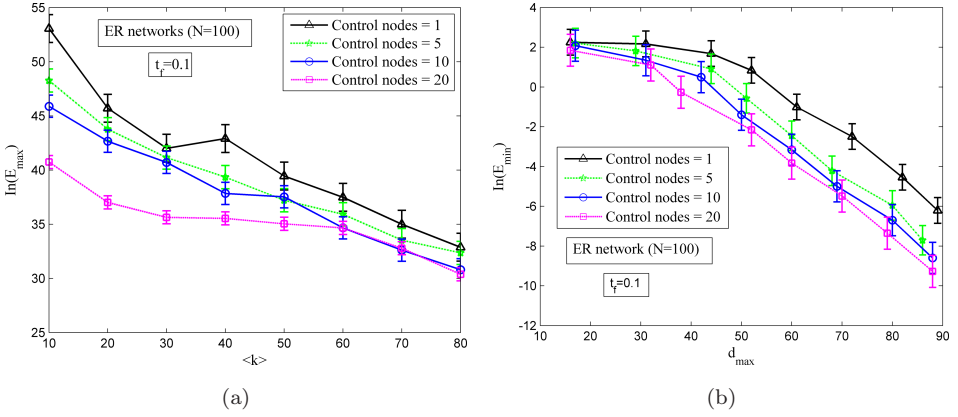


Fig. 9. These two subfigures indicate the relationship between the control energy (E_{\max} and E_{\min}) and the degree ($\langle k \rangle$ or d_{\max}) of nodes in ER networks. Here A is the adjacency matrix, in which we add self-loops as $A_{ii} = \sum_{i,j=1}^n A_{ij}$, and the input control signals directly to control nodes from 1 to N ($N = 1, 5, 10, 20$). (a) E_{\max} as a function of $\langle k \rangle$ with different control nodes and (b) E_{\min} as a function of d_{\max} with different control nodes.

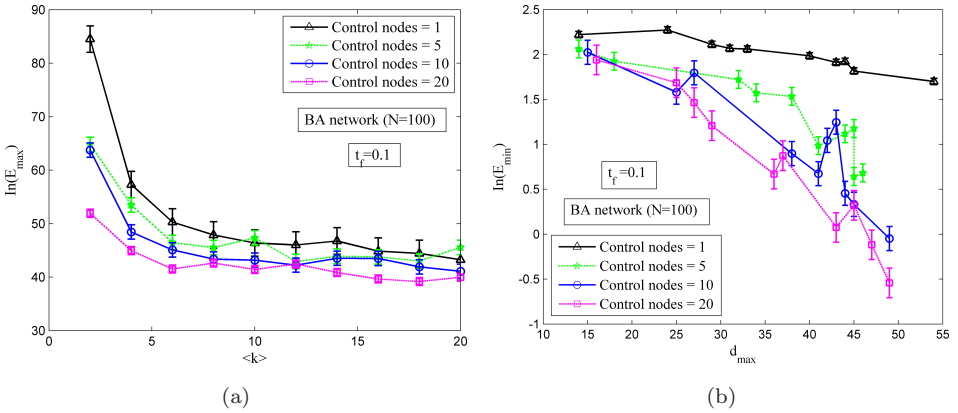


Fig. 10. These two subfigures indicate the relationship between the control energy (E_{\max} and E_{\min}) and the degree ($\langle k \rangle$ or d_{\max}) of nodes in BA networks. Here A is the adjacency matrix, in which we add self-loops as $A_{ii} = \sum_{i,j=1}^n A_{ij}$, and the input control signals directly to control nodes from 1 to N ($N = 1, 5, 10, 20$). (a) E_{\max} as a function of $\langle k \rangle$ with different control nodes and (b) E_{\min} as a function of d_{\max} with different control nodes.

can see that: (1) The maximal energy E_{\max} of ER and BA networks is negatively correlated with the average degree of nodes (Figs. 9(a) and 10(a)). (2) The minimal energy E_{\min} of ER and BA networks is negatively correlated with the maximum degree of nodes (Figs. 9(b) and 10(b)). (3) For ER and BA networks, if the system is completely controllable, the maximal and minimal energy costs are decreased with an increase in the number of control nodes.

5. The Control Strategy of Complex Networks

5.1. Sum of degree of control nodes determines the energy cost

In [15], the structural controllability of complex networks was converted into a maximum matching problem on the network, i.e., we can gain complete control over a directed network if and only if we directly control each unmatched node. But there exists a large number of the maximum matchings in a complex network. In other words, there are many different combinations of control nodes. We simulate five networks, i.e., one simple network, two random networks (ER and BA) and two realistic biological networks (Epithelial to Mesenchymal Transition (EMT) network [31, 20] and p53-mediated DNA damage response network [31, 35]) to elucidate how the sum of degree of control nodes affects the energy cost.

For a simple network with 6 nodes in Fig. 11(a), there are four different maximum matchings (Figs. 11(b)–11(e)), where A is the adjacency matrix. According to Eq. (9), we calculate their maximal and minimal energies depicted in Figs. 12(a) and 12(b), respectively, where A is the adjacency matrix. These results indicate that the combination of control nodes with the higher sum of degree has the lower energy.

For ER and BA random networks with 100 nodes when A is the adjacency matrix, in which we add self-loops as $A_{ii} = \sum_{i,j=1}^n A_{ij}$, they are easily controllable

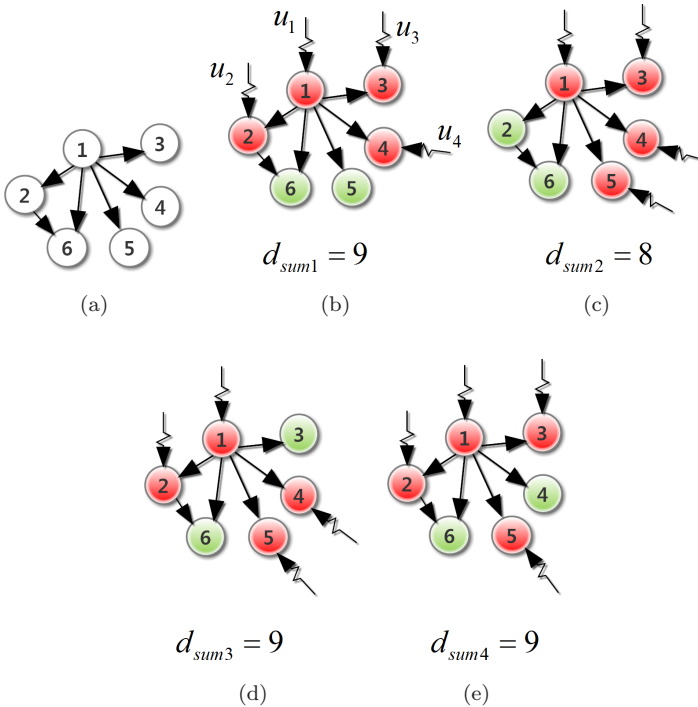


Fig. 11. (a) A simple network with 6 nodes and 6 interactions. (b–e) Four different maximum matchings for this network with different sum of degree d_{sum} .

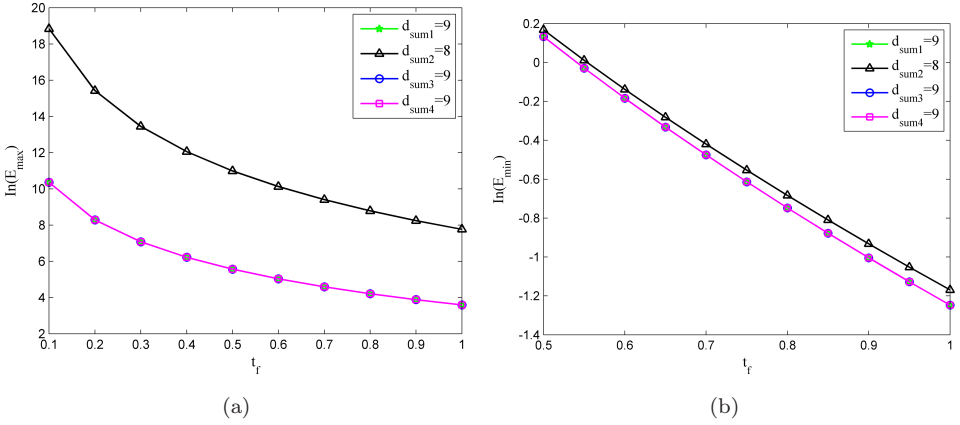


Fig. 12. (a) The maximal energy evolves over control time t_f for four different control node combinations. (b) The minimal energy evolves over control time t_f for four different control node combinations.

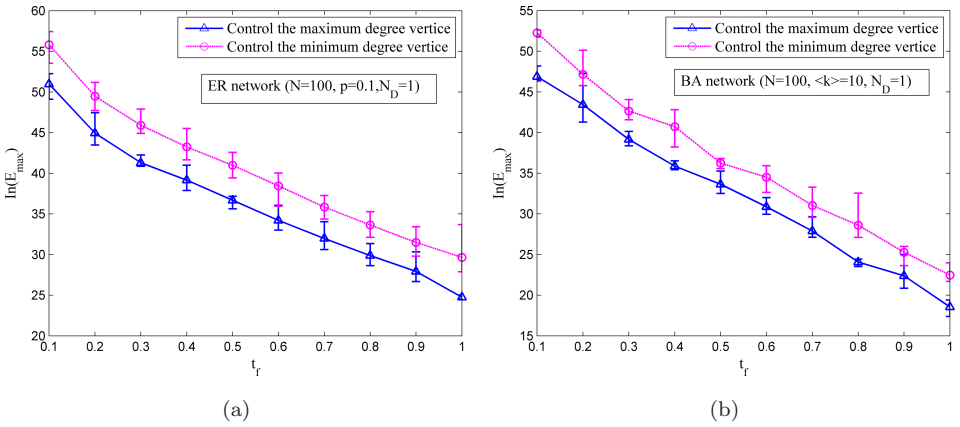


Fig. 13. (a) and (b) indicate the maximal energy evolves with control time t_f for ER and BA networks, respectively.

by anyone of nodes using the method proposed in [15]. We choose to control the node with the maximum degree or the minimum degree, respectively. The results show that the maximal energy with the maximum degree is lower than that with the minimum degree for both of random networks (Figs. 13(a) and 13(b)) and the minimal energy with the maximum degree is also lower than that with the minimum degree for both of random networks (Figs. 14(a) and 14(b)), which are also consistent with results that the energy cost is negatively correlated with the degree of nodes shown in above section.

Furthermore, we explore the energy cost of two realistic biological networks: one is EMT network and another is p53-mediated DNA damage response network (Fig. 15). For these two networks, we obtain three different combinations of control

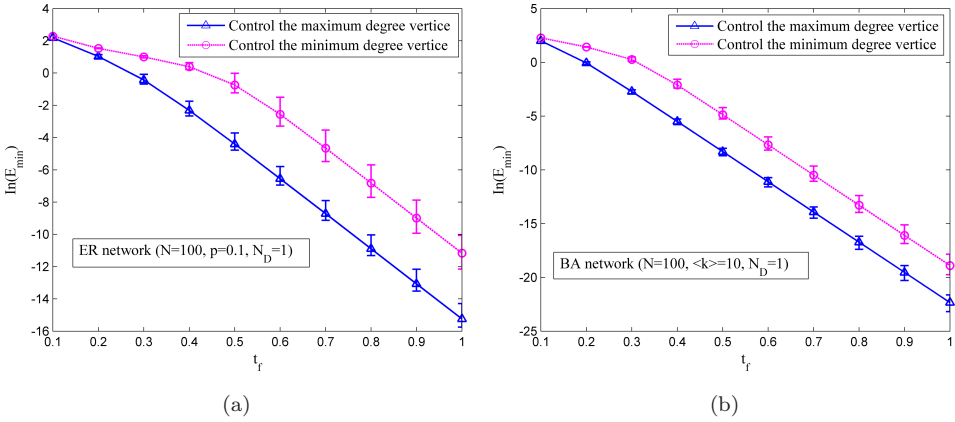


Fig. 14. (a) and (b) indicate the minimal energy evolves with control time t_f for ER and BA networks, respectively.

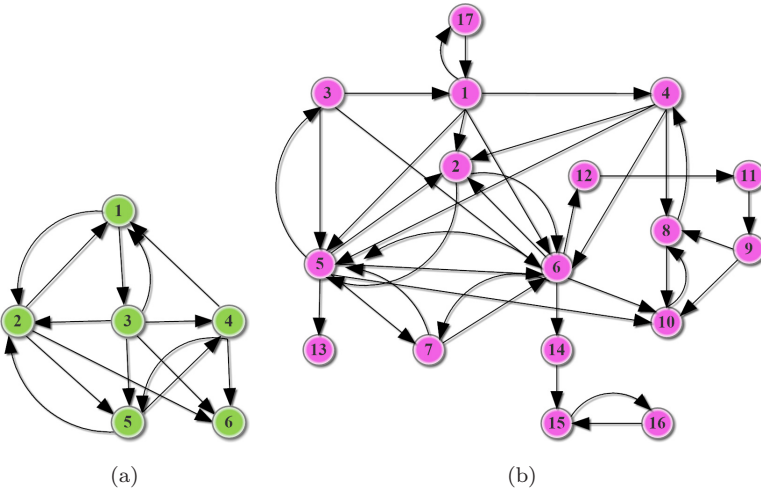


Fig. 15. (a) The EMT network with 6 nodes (1. miR-203; 2. ZEB2; 3. SNAI1; 4. ZEB1; 5. miR-200; 6. CDH1) and 15 interactions. (b) The p53-mediated cell damage response network with 17 molecules (1. ATM*; 2. p53; 3. Wip1; 4. Mdm2n; 5. p53arrestor; 6. p53killer; 7. p53DINP1; 8. Mdm2cp; 9. Akt*; 10. Mdm2c; 11. PIP3; 12. PTEN; 13. P21; 14. p53AIP1; 15. CytoC; 16. Casp3; 17. ATM2) and 40 interactions.

nodes. The sum of degree of all nodes in different combinations is different. In EMT network, three different control sets are (1) ZEB2, miR-200, CDH1 ($d_{sum} = 14$); (2) miR-203, ZEB1, miR-200 ($d_{sum} = 15$); (3) miR-203, ZEB2, miR-200 ($d_{sum} = 16$). In the other network, three control sets are (1) p53killer, PTEN, P21, p53AIP1 ($d_{sum} = 17$); (2) Wip1, p53killer, PTEN, P21 ($d_{sum} = 19$); (3) Wip1, p53killer, p53DINP1,

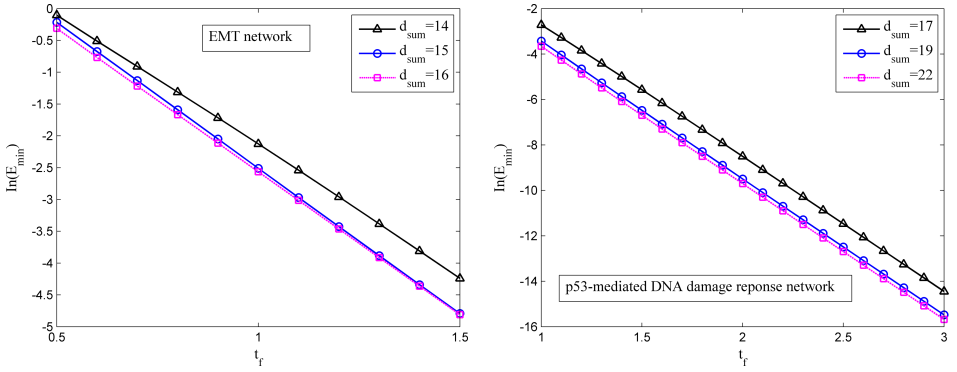


Fig. 16. The minimal energy evolves with control time t_f for EMT network and p53-mediated cell damage response network at three different combinations of control nodes.

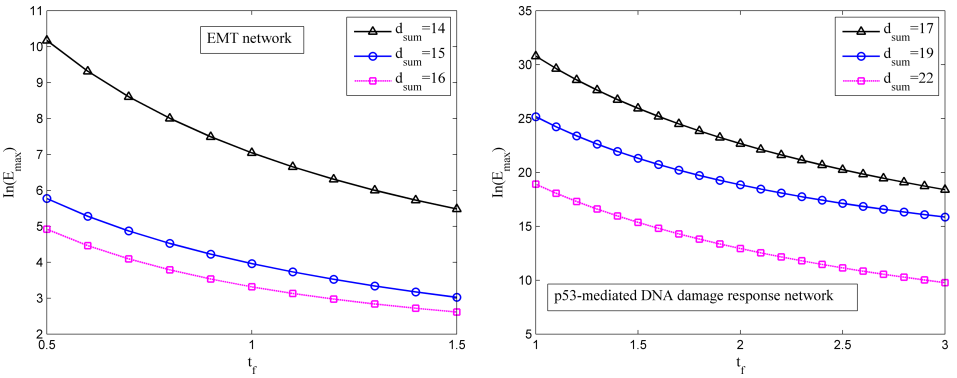


Fig. 17. The maximal energy evolves with control time t_f for EMT network and p53-mediated cell damage response network at three different combinations of control nodes.

Casp3($d_{\text{sum}} = 22$). Figures 16 and 17 further confirm that combinations with higher sum of degree of all nodes have lower maximal energy cost and minimal energy cost.

All together, numerical simulations for five networks indicate that the combinations with the greater sum of degree of control nodes need less energy to implement complete control.

5.2. The multi-objective optimization model for realizing the control with lower energy

The maximum matching problem can be treated by using the cavity method developed in statistical physics [15, 18, 19]. Consider a digraph $G(V, E)$, in order to find a maximum matching M , the goal is to find the minimum $M_G(\{s\})$ that satisfies

the following condition of matching:

$$\sum_{j \in \partial^+ i} s_{(i \rightarrow j)} \leq 1 (i, j \in V), \quad \sum_{k \in \partial^- i} s_{(k \rightarrow i)} \leq 1 (i, k \in V),$$

where ∂^- and ∂^+ indicate the sets of nodes that point to i and are pointed by i , respectively, $M_G(\{s\}) = \sum_{i \in V} M_i(\{s\}) = \sum_{i \in V} (1 - \sum_{k \in \partial^- i} s_{(k \rightarrow i)})$, and $s_{(i \rightarrow j)} \in \{0, 1\}$ assigned to each directed edge or arc $(i \rightarrow j) \in E$ with $s_{(i \rightarrow j)} = 1$ if $(i \rightarrow j) \in M$ and $s_{(i \rightarrow j)} = 0$ otherwise.

Through above numerical simulations for random networks and biological networks, we have found that the greater sum of degree of control nodes is, the less energy is required to implement complete control. Therefore, we consider setting up a control strategy, which not only ensures the fewer control nodes, but also guarantees the less energy cost of control, can be converted into the following multi-objective optimization problem:

$$\begin{aligned} \min M_G(\{s\}) &= \sum_{i \in V} M_i(\{s\}) = \sum_{i \in V} \left(1 - \sum_{k \in \partial^- i} s_{(k \rightarrow i)} \right), \\ \max d_G(\{s\}) &= \sum_{i \in V} d_i M_i(\{s\}), \\ \text{subject to} &\begin{cases} \sum_{j \in \partial^+ i} s_{(i \rightarrow j)} \leq 1 (i, j \in V) \\ \sum_{k \in \partial^- i} s_{(k \rightarrow i)} \leq 1 (i, k \in V) \\ s_{(i \rightarrow j)} \in \{0, 1\} (i, j \in V) \\ s_{(i \rightarrow j)} = 0 \quad \text{if } (i \rightarrow j) \notin E. \end{cases} \end{aligned} \tag{22}$$

We convert this multi-objective optimization model into the following single objective optimization:

$$\begin{aligned} \min \alpha M_G(\{s\}) - \beta d_G(\{s\}) \\ \text{subject to} &\begin{cases} \alpha + \beta = 1, 0 \leq \alpha, \beta \leq 1 \\ \sum_{j \in \partial^+ i} s_{(i \rightarrow j)} \leq 1 (i, j \in V) \\ \sum_{k \in \partial^- i} s_{(k \rightarrow i)} \leq 1 (i, k \in V) \\ s_{(i \rightarrow j)} \in \{0, 1\} (i, j \in V) \\ s_{(i \rightarrow j)} = 0 \quad \text{if } (i \rightarrow j) \notin E. \end{cases} \end{aligned} \tag{23}$$

We use Lingo software to solve this problem. The results are listed in Table 1. From Table 1, we can observe that the obtained combinations with greater sum of degree need less energy cost of control.

Table 1. The relationship among control nodes, the sum of the degree and energy cost for two different biological networks (control time $t_f = 1$).

Different weights	EMT network				p53 network			
	Control nodes	d_{sum}	$\ln(E_{\text{min}})$	$\ln(E_{\text{max}})$	Control nodes	d_{sum}	$\ln(E_{\text{min}})$	$\ln(E_{\text{max}})$
$\alpha = 1, \beta = 0$	{1}	5	-1.70	37.41	{7, 12, 13}	7	-2.18	37.91
$\alpha = 0.9, \beta = 0.1$	{3}	6	-2.44	35.21	{3, 7, 14}	11	-3.19	34.61
$\alpha = 0.8, \beta = 0.2$	{2}	6	-1.92	35.95	{3, 7, 14}	11	-3.19	34.61

6. Conclusion and Discussion

In this study, we have explored the controllability of complex networks from the energy perspective by quantifying with the maximal energy and the minimal energy as measures of network controllability. The main contributions of our work include. (1) By combining theoretical derivation and numerical simulations, we have obtained lower bounds of the maximal and the minimal energy costs for an arbitrary network, which are related to their eigenvalues of state transition matrix. (2) We deduce that controlling unstable networks is easier than controlling stable networks with the same size. (3) We have demonstrated a tradeoff between the control energy and the average degree (or the maximum degree) of an arbitrary undirected network. (4) Numerical simulations have showed that the energy cost has a negative correlation with the degree of nodes. Moreover, the combinations of control nodes with the greater sum of degree requires the less energy to achieve complete control. (5) We have proposed a multi-objective optimization model to obtain the control strategy, which not only ensures the fewer control nodes but also guarantees the less energy cost of control.

There are some important aspects requiring further research, including (1) In Theorem 4.1, we derived a tradeoff between the control energy and the average degree of an arbitrary undirected network in the case that A is positive definite. But we do not have a similar conclusion deduced for the case that A is not positive definite, which needs to be further investigated. (2) In Sec. 5.1, numerical simulations for five networks indicate that the combinations with the greater sum of degree of control nodes need less energy to implement complete control, but we have not deduced it theoretically, which also needs further investigation. (3) In general, many realistic networks are nonlinear [9, 29], so the control of nonlinear dynamical systems is an important topic in the future.

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