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Optimal localization of diffusion sources in complex networks

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Locating sources of diffusion and spreading from minimum data is a significant problem in network science with great applied values to the society. However, a general theoretical framework dealing with optimal source localization is lacking. Combining the controllability theory for complex networks and compressive sensing, we develop a framework with high efficiency and robustness for optimal source localization in arbitrary weighted networks with arbitrary distribution of sources. We offer a minimum output analysis to quantify the source locatability through a minimal number of messenger nodes that produce sufficient measurement for fully locating the sources. When the minimum messenger nodes are discerned, the problem of optimal source localization becomes one of sparse signal reconstruction, which can be solved using compressive sensing. Application of our framework to model and empirical networks demonstrates that sources in homogeneous and denser networks are more readily to be located. A surprising finding is that, for a connected undirected network with random link weights and weak noise, a single messenger node is sufficient for locating any number of sources. The framework deepens our understanding of the network source localization problem and offers efficient tools with broad applications.

1. Introduction

Dynamical processes taking place in complex networks are ubiquitous in natural and in technological systems [1], examples

of which include disease or epidemic spreading in the human society [2,3], virus invasion in computer and mobile phone networks [4,5], behaviour propagation in online social networks [6] and air or water pollution diffusion [7,8]. Once an epidemic or environmental pollution emerges, it is often of great interest to be able to identify its source within the network accurately and quickly so that proper control strategies can be devised to contain or even to eliminate the spreading process. In general, various types of spreading dynamics can be regarded as diffusion processes in complex networks, and it is of fundamental interest to be able to locate the *sources of diffusion*. A straightforward, brute-force search for the sources requires accessibility of global information about the dynamical states of the network. However, for large networks, a practical challenge is that our ability to obtain and process global information can often be quite limited, making brute-force search impractical with undesired or even disastrous consequences. For example, the standard breadth-first search algorithm for finding the shortest paths, when being implemented in online social networks, can induce information explosion even for a small number of searching steps [9]. Recently, in order to locate the source of the outbreak of Ebola virus in Africa, five medical practitioners lost their lives [10]. All these call for the development of efficient methodologies to locate diffusion sources based only on limited, practically available information without the need of acquiring global information about the dynamical states of the entire network.

There were pioneering efforts in addressing the source localization problem in complex networks, such as those based on the maximum-likelihood estimation [11], belief propagation [12], the phenomena of hidden geometry of contagion [13] and inverse spreading [14,15]. In addition, some approaches have been developed for identifying super spreaders that promote spreading processes stemming from sources [16–18]. In spite of these efforts, achieving accurate source localization from a small number of measurements remains challenging. Prior to our work, a systematic framework dealing with the localization of diffusion sources for arbitrary network structures and interaction strength was missing.

In this paper, we develop a theoretical framework to address the problem of network source localization in a detailed and comprehensive way. The main focus is on the fundamental issue of *locatability*, i.e. given a complex network and limited (sparse) observation, are diffusion sources locatable? A practical and extremely challenging issue is, given a network, can a minimum set of nodes be identified which produce sufficient observation so that sources at arbitrary locations in the network can actually be located? To address these issues in a systematic manner, we use a two-step solution strategy. First, we develop a minimum output analysis to identify the minimum number of messenger/sensor nodes, denoted as N_m , to fully locate any number of sources in an efficient way. The ratio of N_m to the network size N , $n_m \equiv N_m/N$, thus characterizes the source locatability of the network in the sense that networks requiring smaller values of n_m are deemed to have a stronger locatability of sources. Our success in offering the minimum output analysis stems from taking advantage of the dual relation between the recently developed controllability theory [19] and the canonical observability theory [20]. Second, given N_m messenger nodes, we formulate the source localization problem as a sparse signal reconstruction problem, which can be solved by using compressive sensing (CS) [21,22], a convex optimization paradigm. The basic properties of CS allow us to accurately locate sources from a small amount of measurement from the messenger nodes, much less than that required in the conventional observability theory. We use our framework to examine a variety of model and real-world networks, and offer analytical prediction of n_m and demonstrate good agreement with numerical calculations. We find that the connection density and degree distribution play a significant role in source locatability, and sources in a homogeneous and denser network are more readily to be located, which differs from existing algorithms for source localization in the literature [11,14,15]. A striking and counter-intuitive finding is that, for an undirected network with one connected component and random link weights, a single messenger node is sufficient to locate any number of sources in the presence of weak noise.

Theoretically, the combination of the minimum output analysis (derived from the controllability and observability theories for complex networks) and the CS-based localization method constitutes a general framework for locating diffusion sources in complex networks. It represents a powerful paradigm to exactly quantify the source locatability of a network and to actually locate the sources efficiently and accurately. Because of the CS-based methodology, our framework is robust against noise [23,24], paving way to practical implementation in noise environment.

2. Results

2.1. A general framework to locate sources with minimum number of messenger nodes

We consider a class of diffusive processes on networks, described by

$$x_i(t+1) = x_i(t) + \beta \sum_{j=1}^N [w_{ij}x_j(t) - w_{ji}x_i(t)]. \quad (2.1)$$

This equation constitutes a good approximation for different types of linear diffusion processes and the linearization of some nonlinear diffusion processes [25]. For example, epidemics can be treated as linear dynamics in the early stages if the network connectivity is high. Variable $x_i(t)$ that denotes the state of node i at time t captures the fraction of infected individuals, the concentration of water or air pollutant, etc., at place i . β is the diffusion coefficient, w_{ij} (w_{ji}) is the weight of the directed link from node j to node i (i to j), ($w_{ij} = w_{ji}$ for undirected networks), and N is the number of nodes in the network (size). It is noteworthy that the value of the diffusion parameter β should be constrained to ensure the physical meaning of $x_i(t)$, i.e. $x_i(t)$ is confined in the range $[0, 1]$ at any time t for any node. We can prove that the confinement of $x_i(t)$ leads to $\beta \in (0, \min_{i=1,2,\dots,N} (1/\sum_{j=1, j \neq i}^N w_{ji}))$ (see electronic supplemental material, S1 for the proof). Equation (2.1) is discrete in time, greatly facilitating computation and analysis. When observations are made from a subset of nodes, the messenger nodes, system (2.1) incorporating outputs from these nodes can be written concisely as

$$\begin{cases} \mathbf{x}(t+1) = (I + \beta L)\mathbf{x}(t), \\ \mathbf{y}(t) = C\mathbf{x}(t), \end{cases} \quad (2.2)$$

where $\mathbf{x}(t) \in \mathbb{R}^N$ is the state vector of the entire network at time t , $I \in \mathbb{R}^{N \times N}$ is the identity matrix, $L = (W - D)$ is a Laplacian matrix, $W \in \mathbb{R}^{N \times N}$ is the weighted adjacency matrix of elements w_{ij} , $D \in \mathbb{R}^{N \times N}$ is a diagonal matrix of elements d_i denoting the total out-weight $\sum_{j \in \Gamma_i} w_{ji}$ of node i , where Γ_i is the neighbouring set of i . The vector $\mathbf{y}(t) \in \mathbb{R}^q$ is the output at time t and $C \in \mathbb{R}^{q \times N}$ is the *output matrix*. Messenger nodes are specified through matrix C and $\mathbf{y}(t)$ records the states of these nodes. The source localization problem is illustrated in figure 1, which is a kind of inverse problem for diffusion and spreading dynamics on complex networks.

The basic difference between source nodes and other nodes in the network is that initially ($t = t_0$), the states of the former are non-zero while those of the latter are zero. To achieve accurate localization of an arbitrary number of sources at arbitrary locations, it is only necessary to recover the initial states of all nodes from the measurements of the messenger nodes at a later time ($t > t_0$). A solution to this problem can be obtained using the observability condition in canonical control theory. To be specific, we consider instants of time: t_0, t_1, \dots, t , and perform a simple iterative process that yields the relation between $\mathbf{x}(t)$ and $\mathbf{x}(t_0)$: $\mathbf{x}(t) = [I + \beta L]^{t-t_0} \mathbf{x}(t_0)$. Consequently, the output, which depends on $\mathbf{x}(t_0)$, can be expressed as $\mathbf{y}(t) = C[I + \beta L]^{t-t_0} \mathbf{x}(t_0)$. The key to accurate localization of sources lies in the existence of a unique solution of the equation, given the output vector $\mathbf{y}(t)$ from the set of messenger nodes as specified by C . Intuitively, to obtain a unique solution, no fewer than N snapshots of measurement are needed. Without loss of generality, we assume that uninterrupted time series from t_0 to $t_0 + N - 1$ are available. We obtain

$$\mathbf{Y} = O \cdot \mathbf{x}(t_0), \quad (2.3)$$

where $\mathbf{Y} \in \mathbb{R}^{qN}$, the initial state vector is $\mathbf{x}(t_0) \in \mathbb{R}^N$, q is the number of messenger nodes, and the matrix $O \in \mathbb{R}^{qN \times N}$ is nothing but the observability matrix in the canonical control theory (see §5.1 for details of equation (2.3)). The observability full rank condition [26] stipulates that, if and only if $\text{rank}(O) = N$, there exists a unique solution of equation (2.3) and the state vector $\mathbf{x}(t_0)$ at initial time t_0 is observable. Insofar as the given output matrix C satisfies the observability rank condition, the initial states of the nodes can be fully reconstructed from the states of the messenger nodes, and all sources can then be located. A challenge is that, in a realistic situation, the initial time t_0 is often unknown, rendering the immediate application of the canonical observability condition invalid. However, a unique and desired feature of our framework is that both $\mathbf{x}(t_0)$ and t_0 can be inferred based on CS (see §§3 and 5.2). Thus, it is possible to develop a theoretical framework on the basis of the observability condition (see electronic supplementary material, S2 for continuous-time processes).

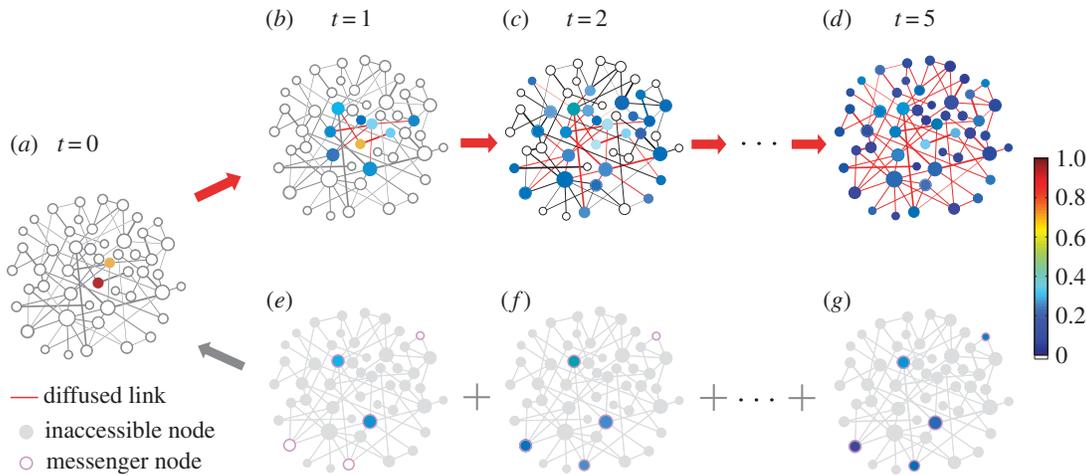


Figure 1. Illustration of source localization problem. (a) A random network with two sources at the initial time $t = 0$. (b–d) The diffusion process at $t = 1$ (b), $t = 2$ (c) and $t = 5$ (d), respectively. The colour bar represents the state of node $x_i(t)$, and those links along which diffusion occurred are marked with red. Panels (a) to (d) describe a diffusion (spreading) process from two sources to the whole network according to equation (2.1). (e–g) Five messenger nodes whose states at three time constants can be measured and collected. The messenger nodes are specified by the output matrix C and the states of messenger nodes and inaccessible nodes constitute $\mathbf{y}(t)$. The time of (e), (f) and (g) corresponds to (b), (c) and (d), respectively. However, in the real situation, the time as well as the initial time is unknown. The only available information for locating sources is the states of a set of messenger nodes at some time and the network structure. (e), (f) and (g) to (a) describe the source localization problem to be solved. Moreover, we aim to identify a minimum set of messenger nodes to locate an arbitrary number of sources at any location by virtue of our minimum output analysis and optimization based on compressive sensing.

2.2. Minimum number of messengers for source localization

Beyond the canonical observability theory, here our goal is to identify a minimum set of messenger nodes to satisfy the full rank condition for observability. However, the brute-force method of enumerating all possible choices of the messenger nodes is computationally prohibitive [27], as the total number of possible configurations is 2^N . Our solution is to use the recently developed, exact controllability framework [19] based on the standard Popov–Belevitch–Hautus (PBH) test theory [28] and to exploit the dual relationship between controllability and observability [20], which results in a practical framework to find the required N_m messenger nodes. In particular, for an arbitrary network, according to the PBH test and the exact controllability framework, N_m is determined by the maximum geometric multiplicity of the eigenvalues λ_i of the matrix $I + \beta L$. After some matrix calculation, we obtain that (see electronic supplementary material, S3)

$$N_m = \max_i \{N - \text{rank}[\lambda_i^L I - L]\}, \quad (2.4)$$

where λ_i^L is the eigenvalue of matrix L and $\mu(\lambda_i^L) \equiv N - \text{rank}[\lambda_i^L I - L]$ is the geometric multiplicity of λ_i^L . It is worth noting that the formula of N_m does not contain the diffusion parameter β , indicating that choices of β do not affect the locatability measure n_m . Equation (2.4) as a result of the standard PBH test is a general minimum output analysis for arbitrary networks.

For an undirected network, L is symmetric and the geometric multiplicity is nothing but the eigenvalue degeneracy. In addition, the eigenvalue degeneracy of L is equal to that of $I + \beta L$ (see electronic supplementary material, S3). Thus, N_m is determined by the maximum eigenvalue degeneracy of L as

$$N_m^{\text{undirect}} = \max_i \{\delta(\lambda_i^L)\}, \quad (2.5)$$

where $\delta(\lambda_i^L)$ is the degeneracy of λ_i^L (the number of appearances of λ_i^L in the eigenvalue spectrum). Equation (2.5) based on the PBH test is our minimum output analysis for arbitrary undirected networks.

Equations (2.4) and (2.5) are the exact theory (ET) for minimum output N_m without any approximations, but the associated computational cost resulting from calculating the eigenvalues and identifying maximum value through a large number of comparisons in equations (2.4) and (2.5) is generally high. Taking advantage of the ubiquitous sparsity of real networks [29], we can obtain an

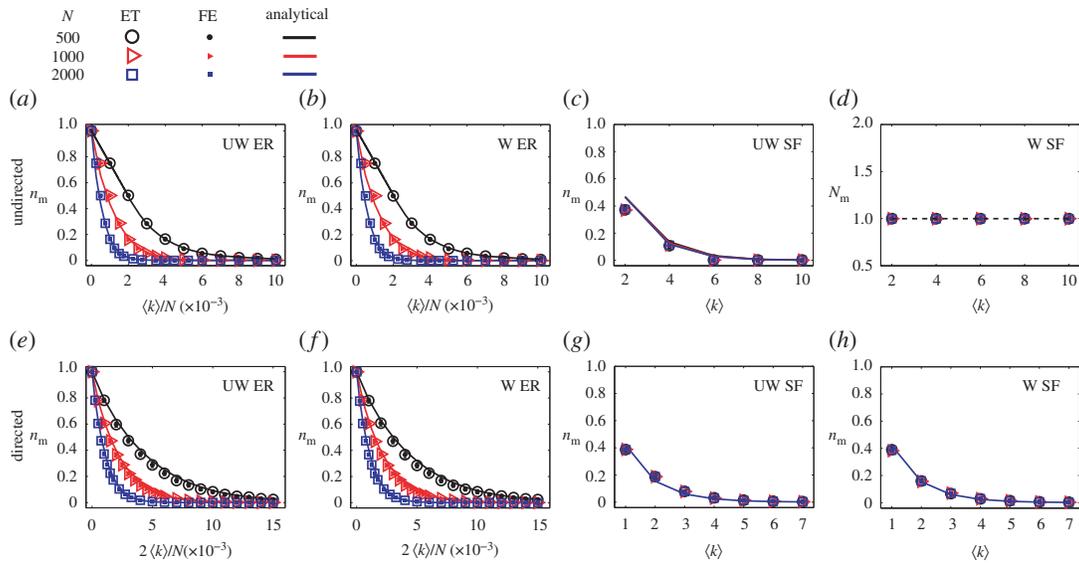


Figure 2. Locatability measure n_m for ER and SF networks. (a–b) For undirected networks, source locatability measure n_m as a function of the connecting probability $\langle k \rangle / N$ for (a) unweighted ER networks and (b) weighted ER networks. (c–d) n_m as a function of the average degree $\langle k \rangle$ for (c) unweighted SF networks, and N_m as a function of the average degree $\langle k \rangle$ for (d) weighted SF networks. For undirected networks, the values of n_m are obtained from the exact theory (ET; equation (2.5)), fast estimation (FE; equation (2.6)), and analytical prediction (Analytical), for different network sizes. The analytical prediction for ER networks is based on equation (2.7). For SF networks in (c), the prediction is from the cavity method. (e–h) For directed networks, source locatability measures n_m as a function of the connecting probability $2 \langle k \rangle / N$ for (e) unweighted and (f) weighted ER networks, and as a function of $\langle k \rangle$ for (g) unweighted and (h) weighted SF networks. For directed networks, the ET results come from equation (2.4), while the FE results for ER and SF networks are from equation (2.6). The analytical predictions for ER and SF networks are from equations (2.8) and (2.9), respectively. For weighted networks, link weights are randomly selected from a uniform distribution in the range (0, 2), which leads to that the mean weight is approximately one. The ET and FE results are obtained by averaging over 50 independent realizations, and the error bars represent the standard deviations. For undirected ER networks, $\langle k \rangle = N p_{\text{con}}$, where p_{con} is the connecting probability between each pair of nodes. Thus, $p_{\text{con}} = \langle k \rangle / N$. For directed ER networks, $\langle k \rangle = N p_{\text{con}} / 2$, yielding $p_{\text{con}} = 2 \langle k \rangle / N$.

alternative method to estimate N_m with much higher efficiency. In particular, for sparse networks, we have (see electronic supplementary material, S4)

$$n_m^{\text{sparse}} \approx 1 - \frac{\text{rank}(aI - L)}{N}, \quad (2.6)$$

where for undirected networks, a is either zero or the diagonal element with the maximum multiplicity (number of appearances in the diagonal) of matrix L . The matrix rank as well as eigenvalues in formula (2.6) can be computed using fast algorithms from computational linear algebra, such as SVD with the computation complexity $O(N^3)$ [30] or LU decomposition with the computation complexity $O(N^{2.376})$ [31]. In general, equation (2.6) allows us to compute n_m efficiently, thereby the term *fast estimation* (FE) method.

2.3. Analytical results for model networks

We first apply our minimum output analysis to undirected Erdős–Rényi (ER) random [32] and scale-free (SF) [33] networks and derive analytical results. Figure 2 shows that, as the average degree $\langle k \rangle$ ($\langle k \rangle \equiv (1/N) \sum_i k_i$, where k_i is the node degree of i) is increased, n_m decreases for undirected ER random networks with identical and random link weights. For the random networks, the efficient formula (2.6) can be further simplified. In particular, for small values of $\langle k \rangle$, due to the isolated nodes and the disconnected components, zero dominates the eigenvalue spectrum of the matrix L [34] where, for example, each disconnected component generates at least one zero eigenvalue in L . For large values of $\langle k \rangle$, we expect all eigenvalues to be distinct without any dominant one. In this case, we can still choose zero to be the eigenvalue associated with a in equation (2.6). Taken together, in a wide range of $\langle k \rangle$ values, the efficient formula equation (2.6) holds with $a = 0$. Alternatively, the value of n_m for ER networks can be theoretically estimated using the degree distribution because of the dominance of the null eigenvalue

(see electronic supplementary material, S4)

$$n_m^{\text{UER}} \approx \begin{cases} 1 - \langle k \rangle / 2 & \langle k \rangle \in [0, 1] \\ \frac{1}{\langle k \rangle} (f(\langle k \rangle) - f(\langle k \rangle)^2 / 2) & \langle k \rangle \in (1, \infty), \end{cases} \quad (2.7)$$

where $f(\langle k \rangle) = \sum_{k=1}^{\infty} (k^{k-1} / k!) (\langle k \rangle e^{-\langle k \rangle})^k$.

For undirected SF networks, a in the efficient formula (2.6) is the diagonal element with the maximum number of appearances in the diagonal of matrix L . In the controllability framework, the density of the driver nodes can be calculated [34,35] with the cavity method [36]. The principle can be extended to analysing locatability measure of SF networks in a similar manner (see electronic supplementary material, S5). The analytical estimation for both ER and SF networks is in good agreement with the results of ET and FE, as shown in figures 2*a–d*. Indeed, the results indicate that choosing $a = 0$ in the efficient formula (2.6) is justified for the ER networks. For small values of $\langle k \rangle$, zero dominates the eigenvalue spectrum, and there are a number of messenger nodes with $n_m > 1/N$. When $\langle k \rangle$ exceeds a certain value, all eigenvalues become distinct, which accounts for the result of a single driver node with $n_m = 1/N$. This relation holds as $\langle k \rangle$ is increased further.

We also find that random link weights have little effect on n_m for ER networks (e.g. comparing figure 2*a* with figure 2*b*), due to the fact that an ER network tends to have many isolated components. By contrast, for SF networks, random link weights can induce a dramatic difference from the case of identical link weights, as shown in figure 2*c* with figure 2*d*. Particularly, a single messenger node is sufficient to locate sources for random link weights with weak noise, regardless of the values of $\langle k \rangle$ and N . This phenomenon can be explained based on equation (2.5), where random link weights can be regarded as imposing perturbation to the eigenvalues of the relevant unweighted Laplacian matrix (the locations of non-zero elements in the two matrices are the same). If the network has a single component, the unweighted Laplacian matrix has only one zero eigenvalue in the spectrum. The random link weights will shift the non-zero eigenvalues in the spectrum, making the probability of finding two or more identical eigenvalues effectively zero. We then expect to find one null eigenvalue and $N - 1$ distinct non-zero eigenvalues so that the entire spectrum contains eigenvalues that are all distinct. As a result, according to equation (2.5), we have $N_m = 1$ for the undirected, single-component SF network with random link weights. A generalization is that, for an arbitrary undirected network with random link weights and multiple components, the value of N_m is exclusively determined by the number of components, N_c , i.e. $N_m = N_c$, due to the fact that each component contributes a null eigenvalue. Consequently, the maximum eigenvalue degeneracy that determines N_m is equal to the number of components, N_c .

We now turn to directed ER and SF networks. For unidirectional links in such a network, the average degree of the network is $\langle k \rangle = \langle k_{\text{out}} \rangle / 2 = \langle k_{\text{in}} \rangle / 2$, where k_{out} and k_{in} denote the out-degree and in-degree, respectively. For directed ER networks, the FE formula is equation (2.6) with $a = 0$. Analytical prediction of n_m can be obtained based on the FE (see electronic supplementary material, S4)

$$n_m^{\text{DER}} \approx e^{-\langle k \rangle} + \frac{\langle k \rangle^2 e^{-2\langle k \rangle}}{4}. \quad (2.8)$$

For directed SF networks, the FE formula is still equation (2.6) with $a = 0, -1$ or -2 (see electronic supplementary material, S4). The quantity n_m can be theoretically predicted via (see electronic supplementary material, S4)

$$n_m^{\text{DSF}} \approx \sum_{k=1}^{N-1} 2^{-k} P(k), \quad (2.9)$$

where k is node degree and $P(k) = P(k_{\text{in}} + k_{\text{out}})$ is the degree distribution. Figure 4*e–h* shows, for directed ER and SF networks, the results of n_m from FE and analytical prediction agree well with those from ET without any approximations.

It is noteworthy that for directed networks with random link weights, N_m is not determined by the number of components, N_c , because there can be more than one zero in the eigenvalue spectrum of a component, a situation that differs from that for undirected networks. In particular, for a directed network, the matrix L can have any number of zero diagonal elements because any node without outgoing links corresponds to such a diagonal element. According to the minimum output analysis, there can then be any number of messenger nodes in a component. As a result, in contrast with undirected

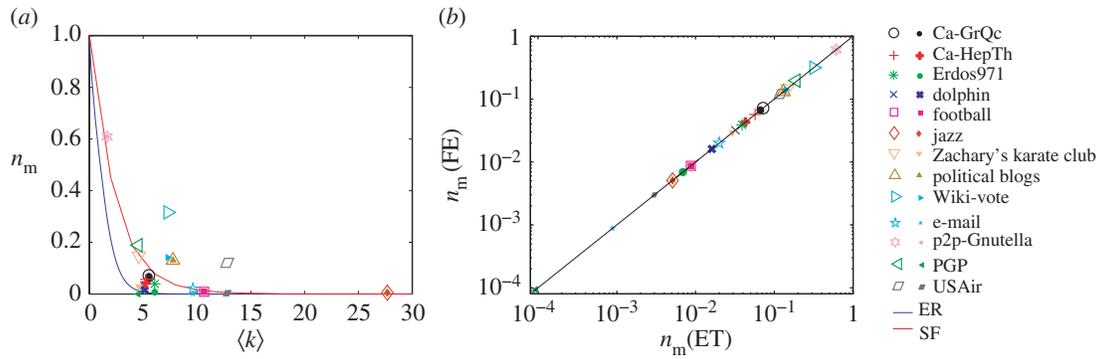


Figure 3. Source locatability of empirical networks. (a) The locatability measure n_m as a function of average degree $\langle k \rangle$ for a number of real social and technological networks, on which diffusion and spreading processes may occur. (b) The locatability measure obtained by using exact theory $n_m(\text{ET})$ (equation (2.4) or equation (2.5)) and obtained by using fast estimation $n_m(\text{FE})$ (equation (2.6)) of real networks. Here, $\langle k \rangle = \langle k_{\text{in}} \rangle / 2 = \langle k_{\text{out}} \rangle / 2$ for a directed network. Theoretical results of ER network (equation (2.7)) and SF network with $\gamma = 3$ (equation (2.9)) are shown as a reference. Hollow symbols represent the results of unweighted real networks and solid symbols represent the results of real networks with random link weights selected from a uniform distribution in the range (0, 2). More details of the real networks can be found in electronic supplementary material, S6 and table S1.

networks with random weights, the quantity N_m in directed networks with random link weights should be calculated by using either equation (2.4) or equation (2.6) for sparse networks, not by counting the number of disconnected components.

2.4. Source locatability of real networks

We also investigate the source locatability n_m for a number of empirical social and technological networks, on which diffusion or spreading processes may occur. Because of the lack of link weights in the real networks, we consider two typical scenarios, unweighted networks and random weight distribution. As shown in figure 3a, n_m for an unweighted real network is always larger than or equal to that of the network with random weights, indicating that random link weights are beneficial to source localization. Another feature is that sources in the technological networks with heterogeneous degree distribution (e.g. Wiki-vote, p2p-Gnutella, PGP, Political blogs, USAir) are usually more difficult to be located than the social networks with relatively homogeneous degree distribution.

We also test the practical feasibility of our fast estimation approaches by using the real networks. As shown in figure 3b, we obtain a good agreement between $n_m(\text{ET})$ based on the exact locatability theory with high computational complexity and $n_m(\text{FE})$ from the fast estimation with much higher efficiency for both unweighted and weighted real networks with random weights. These results validate our fast estimation approach as applied to real networks. (The characteristics of the real networks are described in electronic supplementary material, S6 and table S1).

Combining the results of real and model networks, we discover that the average node degree, the degree distribution and the link weight distribution jointly determine the source locatability. In particular, sources in networks with a homogeneous degree distribution, more connections and random link weights are more readily to be located.

2.5. Identification of messenger node set

We demonstrate how the N_m messenger nodes can be identified using the theory of exact observability of complex networks [19]. In particular, according to the classic PBH test theory [28] and our locatability theory, the output matrix C associated with the N_m messenger nodes satisfies the rank condition $\text{rank}(\lambda^{\max} C - L) = N$, where λ^{\max} is the eigenvalue with the maximum geometric multiplicity $\mu(\lambda^{\max})$ of matrix L , i.e. $N - \text{rank}(\lambda^{\max} I - L)$ reaches maximum value that is nothing but N_m (see equation (2.4); electronic supplementary material, S3). Messenger nodes can be identified insofar as the output matrix C is determined. The computation complexity of our elementary transformation is $O(N^2(\log N)^2)$ [37]. Figure 4a–j illustrates, for an undirected and a directed network, the working of our method of identifying the messengers. For each case, we first compute the eigenvalues λ_i^L of the matrix L and

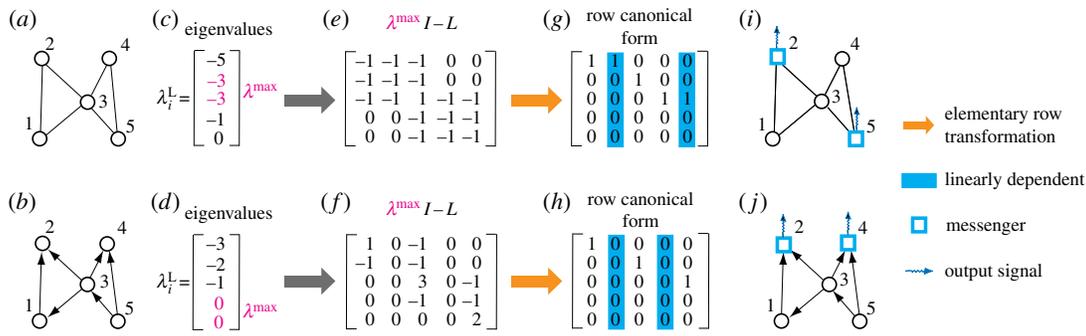


Figure 4. Identification of messengers. (a–b) Illustration of our method to identify messenger nodes for (a) a simple undirected network and (b) a simple directed network. (c–d) Eigenvalues of the undirected network in (a) and that of the directed network in (b), respectively. In (c) and (d), the eigenvalue λ^{\max} corresponding to the maximum geometric multiplicity $\mu(\lambda^{\max})$ is highlighted in red. (e–f) Matrix $\lambda^{\max}I - L$ for the network in (a) and (b), respectively, where λ^{\max} is highlighted. (g–h) Row canonical form of the matrix in (e) and (f) as a result of elementary row transformations, respectively. Here, linearly dependent columns in (g) and (h) are highlighted in blue. (i–j) Messenger nodes corresponding to the linearly dependent columns in the network in (a) and (b), respectively, and output signals produced by messenger nodes. For the network in (a) and (b), the configuration of messengers is not unique as it depends on the elementary row transformation, but the number of messengers N_m is fixed and solely determined by $\mu(\lambda^{\max})$.

find the eigenvalue λ^{\max} corresponding to $\mu(\lambda^{\max})$. We then implement elementary row transformation on $\lambda^{\max}I - L$ to obtain its row canonical form that reveals a set of linearly dependent columns. The messenger nodes are nothing but the nodes corresponding to the columns that are linearly dependent on other columns. The minimum number of messenger nodes (linearly dependent columns) is exactly N_m . Note that alternative configurations of the messenger nodes are possible. For example, as shown in figure 4g, we find that columns 1 and 2, and columns 4 and 5 are linearly correlated, requiring two messengers. As a result, there are four equivalent combinations for the messenger nodes: (1, 4), (1, 5), (2, 4) and (2, 5), any of which can be chosen.

3. Source localization based on compressive sensing

A result from the canonical observability theory is that, in order to fully reconstruct $\mathbf{x}(t_0)$ from solutions of equation (2.3), at least N -step measurements from the messenger nodes are necessary. However, for our localization problem, the sources are ‘minority’ nodes in the sense that the number of sources is much smaller than the network size. In fact, the states of most nodes in the network are zero initially, indicating that the vector $\mathbf{x}(t_0)$ is sparse with a large number of zero elements. The sparsity of $\mathbf{x}(t_0)$ can be exploited to greatly reduce the measurement requirement. In particular, in the CS framework for sparse signal reconstruction [22,38], equation (2.3) can be solved and accurate reconstruction of $\mathbf{x}(t_0)$ can be achieved through solutions of the following convex-optimization problem

$$\min \|\mathbf{x}(t_0)\|_1 \quad \text{subject to } \mathbf{Y} = \mathbf{O} \cdot \mathbf{x}(t_0), \quad (3.1)$$

where $\|\mathbf{x}(t_0)\|_1 = \sum_{i=1}^N |x_i(t_0)|$ is the L_1 norm of $\mathbf{x}(t_0)$, $\mathbf{Y} \in \mathbb{R}^{qM}$, $\mathbf{O} \in \mathbb{R}^{qM \times N}$ and $\mathbf{x}(t_0) \in \mathbb{R}^N$.

If \mathbf{O} satisfies the restricted isometry property (RIP) [39], a full reconstruction of $\mathbf{x}(t_0)$ can be guaranteed theoretically through M -step measurements via some standard optimization method, where M is much smaller than N . For realistic complex networks, the RIP may be violated, but because of the linear independence of rows in matrix \mathbf{O} it is still feasible to reconstruct $\mathbf{x}(t_0)$ from sparse data, where M can still be much smaller than N . Another advantage associated with the CS framework lies in its robustness against noise. Especially, to obtain the direct solution of $\mathbf{x}(t_0)$ is not possible when there is measurement noise or measurements are not sufficient ($M < N$), but the CS framework overcomes these difficulties.

A complete description of our framework to reconstruct the initial states with unknown t_0 is described in §5.2. Here, we present an example of locating diffusion sources in an SF network, as shown in figure 5. For an SF network of a single connected component and random link weights, our minimum output analysis gives $N_m = 1$, and the single messenger node can be selected arbitrarily. As shown in figure 5a for an SF network with four sources and a single messenger node. For convenience, we define data $\equiv M/N$, i.e. the ratio of the utilized amount of measurement to the amount required by the canonical observability

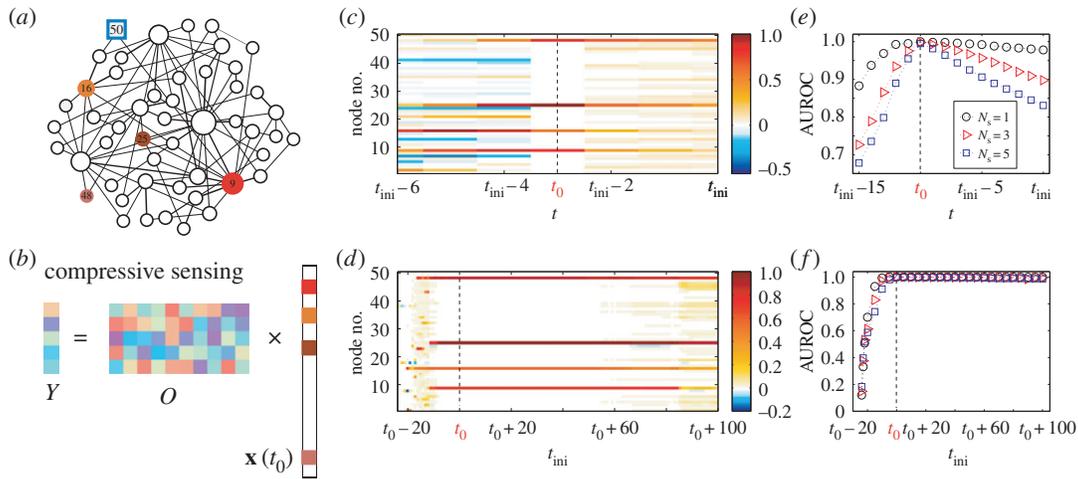


Figure 5. An example of locating sources in undirected weighted SF networks. (a) Illustration of an SF network with four sources with colours representing the initial state values. One messenger node is specified as a blue square. The thickness of the links represents their weight and the sizes of the nodes indicate their degrees. (b) The form of $\mathbf{Y} = \mathbf{O}\mathbf{x}(t_0)$ and the sparse initial state vector $\mathbf{x}(t_0)$ to be reconstructed by using compressive sensing from a relatively small amount of data. (c) Reconstructed state $x_i(t)$ of each node for $t \leq t_{\text{ini}}$, where the initial observation time is t_{ini} ($t_{\text{ini}} \geq t_0$). Colours represent the values of $x_i(t)$ with $t \leq t_{\text{ini}}$. (d) Reconstructed initial state $x_i(t_0)$ of each node from different initial observation time t_{ini} when t_0 , the true triggering time, is being successfully inferred. Colours represent the reconstructed values of $x_i(t_0)$. The colours have the same meanings as those in (a). The four sources are randomly selected and their $x_i(t_0)$ values are larger than zero. (e) Area under a receiver operating characteristic (AUROC) as a function of t ($t \leq t_{\text{ini}}$) for a fixed initial observation time t_{ini} . (f) AUROC versus t for different initial observation time t_{ini} and different number of sources (N_s). Network parameters are set as follows. Network size is $N = 50$, the average degree is $\langle k \rangle = 4$, and the random link weights are selected from a uniform distribution in the range $(0, 2)$. For the diffusion dynamics, we set the diffusion parameter to be $\beta = 0.05$ and the initial state of sources in $\mathbf{x}(t_0)$ is randomly selected from a uniform distribution in the range $(0.1, 1)$. To implement the source localization process, the parameters are: noise amplitude $\sigma = 0$, data = 0.5, and the results are obtained by averaging over 300 independent simulations.

theory. Figure 5b shows the form of $\mathbf{Y} = \mathbf{O}\mathbf{x}(t_0)$, in which the initial state vector $\mathbf{x}(t_0)$ is to be reconstructed. Note that $\mathbf{x}(t_0)$ is quite sparse with four non-zero elements corresponding to the four sources. Thus, $\mathbf{x}(t_0)$ can be reconstructed by using the compressive sensing from a relatively small amount of data. Figure 5c shows, for data = 0.5 and in the absence of noise, four sources and their locations as well as the initial (triggering) time t_0 can be accurately inferred, even though t_0 is unknown. We see that the reconstructed state $\mathbf{x}(t_{\text{ini}} - 3)$ is the sparsest in the sense that it is sparser than all the other states before and after $t_{\text{ini}} - 3$. This indicates that the initial time is $t_0 = t_{\text{ini}} - 3$ and $\mathbf{x}(t_{\text{ini}} - 3)$ is the initial state, in which $x_i(t_{\text{ini}} - 3)$ with non-zero values correspond to sources.

An alternative criterion for inferring initial time t_0 is that $\mathbf{x}(t_0)$ is non-negative but some elements in $\mathbf{x}(t_0 - 1)$ are negative. The presence of negative values in $\mathbf{x}(t_0 - 1)$ is because of the violation of physical process at time $t_0 - 1$. Actually, the diffusion process at $t_0 - 1$ does not exist, such that there is no physical solution of $\mathbf{x}(t_0 - 1)$, regardless of using any methods to solve $\mathbf{x}(t_0 - 1)$. A forced solution of $\mathbf{x}(t_0 - 1)$ will account for unreasonable values in $\mathbf{x}(t_0 - 1)$. As a result, negative values in $\mathbf{x}(t_0 - 1)$, $\mathbf{x}(t_0 - 2)$, ... are highly possible, and offer an alternative way to the sparsity $\mathbf{x}(t)$ for inferring t_0 .

In this manner, not only can we locate the sources but we can also infer the initial states of the source nodes. As shown in figure 5c, the reconstructed initial state values of the sources at $t = t_0$ are in good agreement with those shown in figure 5a (see §5.2 for more details). Figure 5d shows how different initial observation time t_{ini} affects source localization. We find that, in the wide range of t_{ini} from $t_{\text{ini}} = t_0 - 10$ to $t_{\text{ini}} = t_0 + 80$, four sources can be precisely located from a small amount of data. Here, $t_{\text{ini}} < t_0$ indicates that we started to observe messenger nodes prior to the occurrence of the diffusion event from the four sources, which is possible because t_0 is unknown. If t_{ini} is much earlier than t_0 , the spreading process may not occur after M -step measurements, rendering source localization impossible using any method in principle. This accounts for the failure of our method for $t_{\text{ini}} < t_0 - 20$. Also, if t_{ini} is much later than t_0 , computing errors and noise effect will be amplified by using the CS-based optimization, leading to the inaccuracy of source localization, e.g. $t_{\text{ini}} > t_0 + 90$. These issues notwithstanding, our method is quite effective for a vast range of t_{ini} for multiple sources based on sparse data from a minimum number of messenger nodes.

To characterize the performance of our source localization method, we use a standard index from signal processing, the area under a receiver operating characteristic (AUROC) [40,41]. In particular, $\text{AUROC} = 1$ indicates the existence of a threshold that can entirely separate the initial states $\mathbf{x}(t_0)$ of the sources from other nodes in the network, giving rise to perfect localization of sources (see electronic supplementary material, S7 for the detailed definition of AUROC). To give a concrete example, we set $t_{\text{ini}} = t_0 + 10$. Figure 5e shows that the value of AUROC reaches unity at $t_{\text{ini}} - 10$, namely t_0 , demonstrating a nearly perfect localization of sources with different number. The highest reconstruction accuracy at $t = t_0$ corresponds to the highest sparsity of the reconstructed state at t_0 in figure 5c. For $t > t_0$, at an arbitrary time t' , the number of nodes with non-zero states will be larger than the number of sources, because of the diffusion from sources to the other nodes. Thus, one may not distinguish sources from the other nodes based on the reconstructed $\mathbf{x}(t')$, accounting for the lower values of AUROC at t' compared with that at t_0 . On the other hand, consider an arbitrary time t'' with $t'' < t_0$. At t'' , the spreading process has not occurred, and there is no causality between the states at t'' and the observation. When we impose the reconstruction on $\mathbf{x}(t'')$, we cannot obtain the true $\mathbf{x}(t'')$ with all zero elements but a virtual initial state vector with certain errors when compared with $\mathbf{x}(t_0)$. The reconstruction errors will cause more non-zero states on the basis of $\mathbf{x}(t_0)$, inducing a denser state vector than $\mathbf{x}(t_0)$ and therefore lower values of AUROC. The reconstruction errors also explain the fact that the value of AUROC decreases more rapidly for $t < t_0$ than for $t > t_0$. Figure 5f shows the statistical results of figure 5d. We see that AUROC reaches unity when the observation time t_{ini} is about 3 time steps ahead of t_0 , and the AUROC value is nearly unchanged as t_{ini} is further increased, which is consistent with the phenomena shown in figure 5d. (In addition, examples of locating sources in ER networks with and without measurement noise, and in SF networks with measurement noise are presented in electronic supplementary material, S8 and figures S1–S3.) Here, we choose the node number 50, i.e. no. 50, to be the messenger. We also find the different choices of messengers do not affect the result of the sources localization, see electronic supplementary material, S8 and figure S4 for the details. We also investigate effects of the network size on the sources localization, and find that the data will be smaller for a larger network size when AUROC reaches 1, see electronic supplementary material, S8 and figure S5. This is because that the initial state $\mathbf{x}(t_0)$ is sparser when the network size is larger, for a certain AUROC, then the amount of data will be smaller by using CS methods.

We also systematically test the performance of our locatability framework with respect to data requirement and robustness against noise. We assume that measurements are contaminated by white Gaussian noise: $\hat{\mathbf{y}}(t) = \mathbf{y}(t)[I + \mathcal{N}(\mathbf{0}, \sigma^2 I)]$, where $\mathbf{0} \in \mathbb{R}^N$ is zero vector and $I \in \mathbb{R}^{N \times N}$ is the identity matrix, and σ is the standard deviation. The results of AUROC as a function of data for ER and SF networks are shown in figures 6a and 6b, respectively. In the absence of noise ($\sigma = 0$), even for data = 0.1, high values of AUROC can be achieved, e.g. 0.9, especially for SF networks. The value of AUROC exceeds 0.95 when the amount of data is 0.3, and reaches unity for data ≥ 0.5 . The essential feature holds in the presence of noise and for arbitrary values of N_s (see electronic supplementary material, S9 and figure S6). Another finding is that, fewer sources (smaller values of N_s) require less data, due to the fact that a sparser $\mathbf{x}(t_0)$ is induced as a result of smaller N_s and in general, the CS framework requires less data to reconstruct a sparser vector. Systematic results on noise resistance are shown in figures 6c–d, where we see that the AUROC value is nearly indistinguishable across different numbers of sources, N_s . This is different from the results in figure 6a,b, and there is almost no difference between the results from ER and SF networks. Figure 6c,d also shows that, as σ is increased from 0 to 1, the AUROC value is only slightly reduced (AUROC ≈ 0.85 for $\sigma = 1$), indicating the extraordinary robustness of our locatability framework against noise. We also study the effect of the diffusion parameter β on source localization with respect to different data amounts and values of the noise variance. We find that β has little influence on the accuracy of source localization (see electronic supplementary material, S10 and figures S7–S9).

4. Discussion

We developed a framework for locating sources of diffusion or spreading dynamics in arbitrary complex networks (directed or undirected, weighted or unweighted) based solely on sparse measurement from a minimum number of messenger nodes. The key to the general framework lies in combining the controllability theory of complex networks with the compressive sensing paradigm for sparse signal reconstruction, both being active areas of research in network science and engineering. Particularly, the minimum set of messenger nodes can be identified efficiently using the minimum output analysis

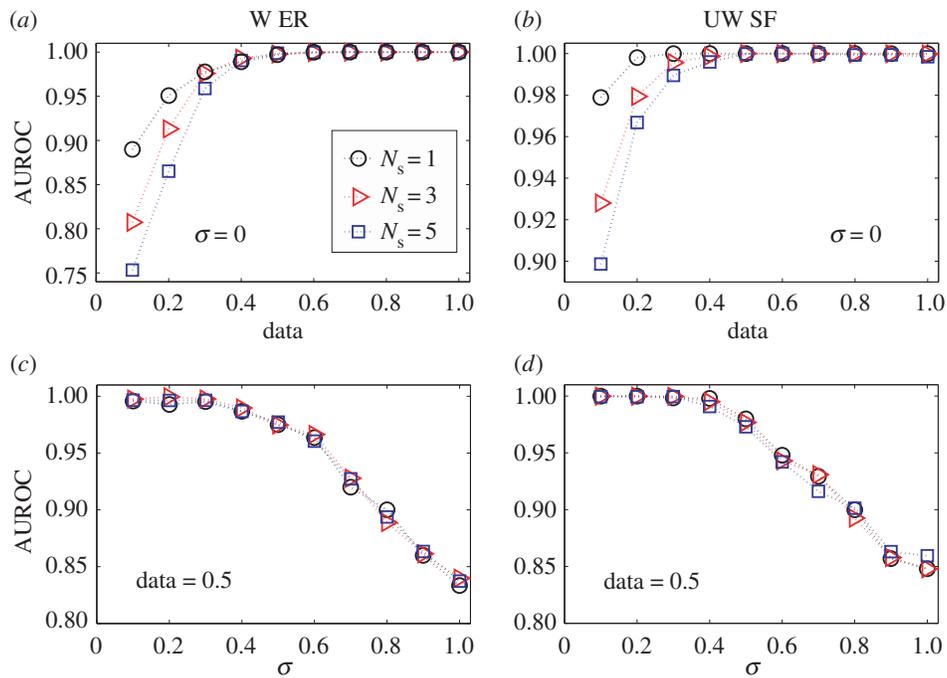


Figure 6. Locatability performance in undirected ER and SF networks. (a–d) AUROC as a function of data for (a) weighted ER and (b) unweighted SF networks, and as a function of noise variance σ for (c) weighted ER and (d) unweighted SF networks. In (a) and (b), σ is fixed at 0. In (c) and (d), data are fixed at 0.5. Cases with different numbers of sources, N_s , are included. For a random guess, the AUROC value is 0.5. The average degree (k) is 2 and 4 for the ER and SF networks, respectively. We set $\beta = 0.1$ for ER networks and $\beta = 0.05$ for SF networks. The results are obtained by averaging over 500 independent simulations. The other parameters are the same as in figure 5.

based on exact controllability of complex networks and the dual relation between controllability and observability. The ratio of the minimum messenger nodes to the network size characterizes the source locatability of complex networks. We find that sources in a denser and homogeneous network are more readily to be located, which distinguishes our work from those in the literature based on alternative algorithms. A finding is that, for undirected networks with one component, random link weights and weak noise, a single messenger node is sufficient to locate sources at any locations in the network. By using the data from the minimum set of messenger nodes, an approach based on compressive sensing is offered to precisely infer the initial time, at which the diffusion process starts, and the sources with non-zero states initially. Because the initial state vector to be recovered for source localization is generically sparse, compressive sensing can be employed to locate the sources from small amounts of measurement, making our framework robust against insufficient data and noise. Practically, the highlights of our framework consist of the following three features: minimum messenger nodes, sparse data requirement and strong noise resistance, which allow the sources of dynamical processes to be identified accurately and efficiently.

Our approach was partially inspired by the pioneering effort in connecting the conventional observability theory for canonical linear dynamical systems with the compressive sensing approach [42–44]. To our knowledge, the source locatability problem has not been tackled in such a comprehensive way prior to our work. The minimal output analysis based on the controllability and observability theory for complex networks deepens our understanding of the dynamical processes on complex networks, which finds applications, e.g. in the design and analysis of large-scale sensor networks. Incorporating compressive sensing to uncover the sources and the original time of diffusion represents an innovative approach to a practical problem of significant interest but limited by finite resources for collecting data and by measurement or background noise. The underlying principle of the framework can potentially be applied to solving other optimization problems in complex networks. While we study diffusion models on time-invariant complex networks, our general framework provides significant insights into the open problem of developing source localization methods for time-variant complex networks hosting nonlinear diffusion processes.

5. Methods

5.1. The main localization formula

The detailed form of $\mathbf{Y} = \mathbf{O} \cdot \mathbf{x}(t_0)$ is

$$\begin{pmatrix} \mathbf{y}(t_0) \\ \mathbf{y}(t_0 + 1) \\ \vdots \\ \mathbf{y}(t_0 + N - 1) \end{pmatrix} = \begin{pmatrix} \mathbf{C} \\ \mathbf{C}[\mathbf{I} + \beta\mathbf{L}] \\ \vdots \\ \mathbf{C}[\mathbf{I} + \beta\mathbf{L}]^{N-1} \end{pmatrix} \mathbf{x}(t_0), \quad (5.1)$$

where N time steps of measurements are necessary to ensure full rank of the observability matrix \mathbf{O} . Insofar as \mathbf{O} is of full rank, according to the canonical observability theory, there exists a unique solution of the initial states to the main localization function.

5.2. Reconstruction of initial state $\mathbf{x}(t_0)$ without knowledge of initial time t_0

For realistic diffusive processes on networks, the initial time t_0 is usually not known *a priori*, making inference of the initial state $\mathbf{x}(t_0)$ a challenging task. Taking advantage of the sparsity of the initial vector $\mathbf{x}(t_0)$ and the underlying principle of compressive sensing, we articulate an effective method to uncover both $\mathbf{x}(t_0)$ and t_0 from limited measurements.

Say the initial observation time is t_{ini} ($t_{\text{ini}} \geq t_0$). Considering all possible t_0 ahead of t_{ini} , we need to reconstruct a series of states, i.e. $\mathbf{x}(t_{\text{ini}})$, $\mathbf{x}(t_{\text{ini}} - 1)$, \dots , $\mathbf{x}(t'_0)$ to ensure that the actual t_0 lies in between t_{ini} and t'_0 . The series of states can be reconstructed from the uninterrupted observation $\mathbf{y}(t_{\text{ini}}), \dots, \mathbf{y}(t_{\text{ini}} + N - 1)$ according to the following equations:

$$\begin{pmatrix} \mathbf{y}(t_{\text{ini}}) \\ \mathbf{y}(t_{\text{ini}} + 1) \\ \vdots \\ \mathbf{y}(t_{\text{ini}} + N - 1) \end{pmatrix} = \begin{pmatrix} \mathbf{C} \\ \mathbf{C}[\mathbf{I} + \beta\mathbf{L}] \\ \vdots \\ \mathbf{C}[\mathbf{I} + \beta\mathbf{L}]^{N-1} \end{pmatrix} \mathbf{x}(t_{\text{ini}}),$$

$$\begin{pmatrix} \mathbf{y}(t_{\text{ini}}) \\ \mathbf{y}(t_{\text{ini}} + 1) \\ \vdots \\ \mathbf{y}(t_{\text{ini}} + N - 1) \end{pmatrix} = \begin{pmatrix} \mathbf{C}[\mathbf{I} + \beta\mathbf{L}] \\ \mathbf{C}[\mathbf{I} + \beta\mathbf{L}]^2 \\ \vdots \\ \mathbf{C}[\mathbf{I} + \beta\mathbf{L}]^N \end{pmatrix} \mathbf{x}(t_{\text{ini}} - 1)$$

$$\vdots$$

and

$$\begin{pmatrix} \mathbf{y}(t_{\text{ini}}) \\ \mathbf{y}(t_{\text{ini}} + 1) \\ \vdots \\ \mathbf{y}(t_{\text{ini}} + N - 1) \end{pmatrix} = \begin{pmatrix} \mathbf{C}[\mathbf{I} + \beta\mathbf{L}]^{t_{\text{ini}} - t'_0} \\ \mathbf{C}[\mathbf{I} + \beta\mathbf{L}]^{t_{\text{ini}} - t'_0 + 1} \\ \vdots \\ \mathbf{C}[\mathbf{I} + \beta\mathbf{L}]^{t_{\text{ini}} - t'_0 + N - 1} \end{pmatrix} \mathbf{x}(t'_0).$$

The reconstruction process is terminated and t_0 can be inferred if a sparsest state is identified, say $\mathbf{x}(t_1)$, i.e. $\mathbf{x}(t_1)$ is sparser than all reconstructed states at time before and after t_1 . Then, $\mathbf{x}(t_1)$ is taken as the initial state with the initial time $t_0 = t_1$.

By exploiting the natural sparsity of $\mathbf{x}(t)$, the CS framework for sparse signal reconstruction allows us to reconstruct $\mathbf{x}(t_{\text{ini}})$, $\mathbf{x}(t_{\text{ini}} - 1)$, \dots , $\mathbf{x}(t'_0)$ iteratively from a small amount of data, i.e. M -step measurements and $M < N$, i.e. $\mathbf{Y} \in \mathbb{R}^{qM}$, $\mathbf{O} \in \mathbb{R}^{qM \times N}$ and $\mathbf{x}(t'_0) \in \mathbb{R}^N$. By contrast, at least N -step measurements are required in the conventional observability theory (equation (5.2)), where M depends on the sparsity of the state vector. In general, M can be much smaller than N , insofar as the number of sources N_s is much smaller than the network size N . According to equations (3.1) and (5.2), $\mathbf{x}(t_{\text{ini}})$, $\mathbf{x}(t_{\text{ini}} - 1)$, \dots , $\mathbf{x}(t'_0)$ can be reconstructed efficiently from a small amount of observation that is much smaller than that required in the conventional observability theory.

Data accessibility. Data can be accessed at <http://sss.bnu.edu.cn/%7Ewenxu/w/data%5fset.htm>.

Authors' contributions. W.-X.W. and Y.-C.L. devised the research project. Z.-L.H. and X.H. performed numerical simulations. W.-X.W., Y.-C.L., Z.-L.H. and X.H. analysed the results. W.-X.W. and Y.-C.L. wrote the paper. All authors gave final approval for publication.

Competing interests. We declare we have no competing interests.

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SUPPLEMENTARY MATERIALS

Optimal Localization of Diffusion Sources in Complex Networks

Zhao-Long Hu, Xiao Han, Ying-Cheng Lai, Wen-Xu Wang

I. Locating sources in continuous-time dynamical networks

A linear, time-invariant, and continuous-time dynamical network system can be described in the following state-space form

$$\begin{cases} \dot{\mathbf{x}}(t) = A\mathbf{x}(t) \\ \mathbf{y}(t) = C\mathbf{x}(t), \end{cases} \quad (\text{S1})$$

where $\mathbf{x}(t) \in \mathbb{R}^N$ represents the complete state of the network system at time t , N is the number of nodes, $\mathbf{y}(t)$ is the vector of q outputs at time t , $A \in \mathbb{R}^{N \times N}$ is the system matrix, and $C \in \mathbb{R}^{q \times N}$ is the output matrix. If the full initial state of the system, $\mathbf{x}(t_0)$, can be obtained from the outputs in the time interval $[t_0, t]$, the system is observable [S1].

To be concrete, we present a general method of reconstructing the initial states of an arbitrary linear time-invariant network using the diffusion model

$$\dot{x}_i(t) = \beta \sum_{j=1}^N [w_{ij}x_j(t) - w_{ji}x_i(t)], \quad (\text{S2})$$

where $x_i(t)$ is the state of node i at the time t , β is the diffusion coefficient (constant), and w_{ij} (w_{ji}) is the weight of a directed link from node j to i (i to j). Combining Eqs. (S2) and (S1), we have

$$\begin{cases} \dot{\mathbf{x}}(t) = \beta L\mathbf{x}(t) \\ \mathbf{y}(t) = C\mathbf{x}(t), \end{cases} \quad (\text{S3})$$

where $L = (W - D)$, $W \in \mathbb{R}^{N \times N}$ is the adjacency matrix of elements w_{ij} , $D \in \mathbb{R}^{N \times N}$ is the diagonal matrix with element d_i representing the total out-weight $\sum_{j \in \Gamma_i} w_{ji}$ of node i (Γ_i is the set of neighbors of node i). The output response of the system is

$$\mathbf{y}(t) = Ce^{\beta L(t-t_0)}\mathbf{x}(t_0). \quad (\text{S4})$$

For convenience, we can stack all the outputs $\mathbf{y}(t)$ into a vector: $\mathbf{Y} = [\mathbf{y}(t_0), \dots, \mathbf{y}(t_0+0.1), \dots, \mathbf{y}(t_0+$

$0.2), \dots, \mathbf{y}(t_0 + t)]^T$. Intuitively, N snapshot measurements of the network state are needed to achieve a unique solution. Without loss of generality, we sample the same time interval T to obtain

$$\begin{pmatrix} \mathbf{y}(t_0) \\ \mathbf{y}(t_0 + T) \\ \vdots \\ \mathbf{y}(t_0 + (N-1)T) \end{pmatrix} = \begin{pmatrix} C \\ Ce^{\beta LT} \\ \vdots \\ Ce^{(N-1)\beta LT} \end{pmatrix} \mathbf{x}(t_0) = O \cdot \mathbf{x}(t_0), \quad (\text{S5})$$

where the matrix $O \in \mathbb{R}^{qN \times N}$ is the so-called observability matrix in canonical control theory. A unique solution of Eq. (S5) exists and the state vector $\mathbf{x}(t_0)$ at initial time is observable if and only if the rank condition $\text{rank}(O) = N$ is satisfied [S2]. Our goal is to identify the minimum set of messenger nodes to satisfy the observability full rank condition.

To achieve our goal, we exploit the recently developed exact controllability theory [S1] and the duality between controllability and observability [S2], which enables us to find N_m , the minimum number of messengers in an efficient manner. In particular, for an arbitrary network, N_m is determined by the maximum geometric multiplicity $\max_i \{\mu(\lambda_i^L)\}$ of the eigenvalues λ_i^L of matrix L , as

$$N_m = \max_i \{N - \text{rank}[\lambda_i^L I - L]\}, \quad (\text{S6})$$

which is exactly the same as that for discrete-time dynamical networks studied in the main text. Insofar as N_m is determined, the key to source localization is then to identify messengers to obtain the output matrix C . The method of identifying messengers is essentially the same as that for the discrete time case: by using the Popov-Belevitch-Hautus (PBH) test theory [S3], we obtain the output matrix C associated with N_m messenger nodes through $\text{rank} \begin{pmatrix} \lambda^{\max} I - L \\ C \end{pmatrix} = N$, where λ^{\max} is the eigenvalue corresponding to the maximum geometric multiplicity $\mu(\lambda^{\max})$ of matrix L . To determine the output matrix C , we implement elementary row transformation on matrix $\lambda^{\max} I - L$ to obtain the row canonical form of the matrix. The nodes whose numbers correspond to the linearly-dependent columns are the messenger nodes. Finally, combining with Eq. (S5), we can locate sources in continuous-time dynamic networks.

Therefore, our theoretical framework of source localization, including the minimum output theory for determining a minimum set of messenger nodes and identifying the messenger nodes is exactly the same for both discrete and continuous dynamical network systems.

II. Proof of the minimum output theory

According to the exact controllability theory [S4] and the dual relation between network controllability and observability [S1], for system (2) in the main text, N_m is determined by the maximum geometric multiplicity of the eigenvalue λ_i of the matrix $I + \beta L$, i.e.,

$$N_m = \max_i \{N - \text{rank}[\lambda_i I - (I + \beta L)]\}. \quad (\text{S7})$$

We can prove that N_m is independent of β in the sense that β can be eliminated from Eq. (S7). For matrix $I + \beta L$, we have

$$\begin{aligned} (I + \beta L)\mathbf{v} &= \mathbf{v} + \beta L\mathbf{v}, \\ &= \mathbf{v} + \beta \lambda_i^L \mathbf{v}, \\ &= (1 + \beta \lambda_i^L)\mathbf{v}, \end{aligned} \quad (\text{S8})$$

where λ_i^L is the eigenvalue of matrix L and \mathbf{v} is the associated eigenvector. Equation (S8) gives the eigenvalue λ_i of matrix $I + \beta L$, i.e.,

$$\lambda_i = 1 + \beta \lambda_i^L. \quad (\text{S9})$$

Inserting the expression of λ_i into Eq. (S7), we have

$$\begin{aligned} N_m &= \max_i \{N - \text{rank}[(1 + \beta \lambda_i^L)I - (I + \beta L)]\}, \\ &= \max_i \{N - \text{rank}[\beta(\lambda_i^L I - L)]\}, \\ &= \max_i \{N - \text{rank}[\lambda_i^L I - L]\}, \end{aligned} \quad (\text{S10})$$

which indicates that the minimum output N_m is independent of the value of β . The exact minimum output theory for arbitrary network [Eq. (5) in the main text] is proved.

For system (2) in the main text with an arbitrary undirected network, according to the exact controllability theory [S4] and the dual relation between network controllability and observability, N_m is determined by the maximum eigenvalue degeneracy of matrix $I + \beta L$, i.e.,

$$N_m = \max_i \{\delta(\lambda_i)\}, \quad (\text{S11})$$

where $\delta(\lambda_i)$ is the eigenvalue degeneracy of matrix $I + \beta L$. Equation (S9) demonstrates that there is a one-to-one correspondence between the eigenvalue λ_i of matrix $I + \beta L$ and the eigenvalue λ_i^L of matrix L . Thus, $I + \beta L$ and L have exactly the same eigenvalue degeneracy, which yields the exact minimum output theory [Eq. (6) in the main text] for undirected networks, i.e.,

$$N_m^{\text{undirect}} = \max_i \{\delta(\lambda_i^L)\}, \quad (\text{S12})$$

and the diffusion parameter β is eliminated.

Furthermore, Eq. (S10) indicates that the geometric multiplicity of the eigenvalues of L is equal to that of $I + \beta L$, and the output matrix C of L is identical to that of $I + \beta L$ as well. Utilizing the Popov-Belevitch-Hautus (PBH) test theory [S3], we can get the output matrix C from

$$\text{rank} \begin{pmatrix} \lambda^{\max} I - L \\ C \end{pmatrix} = N, \quad (\text{S13})$$

instead of

$$\text{rank} \begin{pmatrix} \hat{\lambda}^{\max} I - (I + \beta L) \\ C \end{pmatrix} = N, \quad (\text{S14})$$

where $\hat{\lambda}^{\max}$ is the maximum geometric multiplicity of the eigenvalues of $I + \beta L$. This implies that the diffusion parameter β has no influence on identifying messenger nodes based on PBH test as well, as described in the subsection *Identification of messenger node set*.

III. Analytical treatment of locatability of ER and SF networks

In general, for an undirected network (symmetric matrix), eigenvalue degeneracy is exactly the same as its geometric multiplicity. Thus, according to the ET formulas, e.g., Eqs. (5) and (6) in the main text, the eigenvalue λ^{\max} with the maximum geometric multiplicity in Eq. (5) is nothing but the eigenvalue with the maximum degeneracy (the number of appearances in the eigenvalue spectrum). In this regard, if we are able to evaluate the eigenvalue with the maximum degeneracy a priori, the calculation of the all eigenvalues in Eq. (6) and that of matrix ranks for all possible eigenvalues in Eq. (5) can be saved, leading to a fast estimation of n_m by inserting the estimated eigenvalue into Eq. (5).

For a sparse undirected network (symmetric matrix), the diagonal elements of the network matrix often dominate eigenvalue spectrum [S5]. Hence, the diagonal elements with the maximum multiplicity (the largest number of appearances in the diagonal) could be a proxy of the eigenvalue with maximum degeneracy. However, for Laplacian matrix L , in addition to the diagonal elements, zero could dominate eigenvalue spectrum as well in the absence of any zero diagonal elements, because of the existence of isolated components. Note that each isolated component or node will contribute one null eigenvalue to the eigenvalue spectrum of a Laplacian matrix. Thus, diagonal elements and zero are possible candidates for formulating a fast estimation of the source locatability measure n_m :

$$n_m^{\text{sparse}} \approx 1 - \frac{\text{rank}(aI - L)}{N}, \quad (\text{S15})$$

where a is either zero or the diagonal element of L with the maximum multiplicity.

In an undirected ER network with small connection probability, there are a number of isolated nodes and isolated components, accounting for the dominance of zero in the eigenvalue spectrum. Thus, the source locatability n_m can be estimated by examining the isolated nodes without links and the nodal pairs. Using the degree distribution $P(k)$ of ER networks, $e^{-\langle k \rangle} \langle k \rangle^k / k!$, we have

$$n_m^{\text{UER}} \approx \max\{1/N, P(k=0) + P(k=1)^2\}, \quad (\text{S16})$$

which gives

$$n_m^{\text{UER}} = \delta(0) \approx e^{-\langle k \rangle} + \langle k \rangle^2 e^{-2\langle k \rangle}. \quad (\text{S17})$$

For a directed network, let k_{out} and k_{in} be the out-degree and in-degree, respectively, and suppose that the links are unidirectional. The average degree of the network is $\langle k \rangle = \langle k_{\text{out}} \rangle / 2 = \langle k_{\text{in}} \rangle / 2$. A fast

estimation of the source locatability yields

$$n_m^{\text{sparse}} \approx 1 - \frac{\text{rank}(aI - L)}{N}, \quad (\text{S18})$$

where a is 0, -1 or -2, due to the fact that the diagonal element of matrix L is dominated by 0, -1 or -2 for small average degree $\langle k \rangle$. Numerical calculations suggest that the main contributions to n_m come from eigenvalues 0, -1 and -2.

For a directed ER network with a small connection probability $2\langle k \rangle/N$, analogous to the undirected case, we only need to consider isolated nodes and nodal pairs to obtain

$$n_m^{\text{DER}} \simeq \max\{1/N, P(k_{\text{out}} = 0, k_{\text{in}} = 0) + P(k_{\text{out}} = 1, k_{\text{in}} = 0)P(k_{\text{out}} = 0, k_{\text{in}} = 1)\}. \quad (\text{S19})$$

Since k_{in} is independent of k_{out} , we have

$$n_m^{\text{DER}} \approx e^{-\langle k \rangle} + \frac{\langle k \rangle^2 e^{-2\langle k \rangle}}{4}. \quad (\text{S20})$$

For a directed SF network, nodes of zero out-degree must be the messengers. In this case, we can estimate n_m as

$$n_m^{\text{DSF}} \simeq \max\{1/N, \sum_m^{N-1} P(k_{\text{out}} = 0|k)P(k)\}, \quad (\text{S21})$$

where $P(k) = P(k_{\text{in}} + k_{\text{out}})$ follows a power law, and $P(k_{\text{out}}|k)$ is the conditional probability that one node has out-degree k_{out} when its degree is k . According to binomial theorem, we have

$$P(k_{\text{out}}|k) = \binom{k}{k_{\text{out}}} \left(\frac{1}{2}\right)^{k_{\text{out}}} \left(\frac{1}{2}\right)^{k-k_{\text{out}}}, \quad (\text{S22})$$

which yields

$$P(k_{\text{out}} = 0|k) = 2^{-k} \quad (\text{S23})$$

and consequently,

$$n_m^{\text{DSF}} \approx \sum_{k=m}^{N-1} 2^{-k} P(k). \quad (\text{S24})$$

IV. Cavity method for estimating locatability

In Ref. [S6], the cavity method was used to quantify the network controllability via the density of the driver nodes for directed networks. The method was subsequently extended to undirected networks [S4]. Because of the duality between controllability and observability, we can use the cavity method to estimate the locatability n_m for general complex networks. In particular, for a directed network with similar in- and out-degree distribution $P(k)$, the locatability n_m is given by

$$n_m = G(w_2) + G(1 - w_1) - 1 + \langle k \rangle w_1(1 - w_2), \quad (\text{S25})$$

where $G(x)$ is the generating function satisfying

$$G(x) = \sum_{k=0}^{\infty} P(k)x^k. \quad (\text{S26})$$

The quantities w_1 and w_2 in Eq. (S25) can be obtained through the following self-consistent equations:

$$w_1 = H[1 - H(1 - w_1)], \quad (\text{S27})$$

$$w_2 = 1 - H[1 - H(w_2)], \quad (\text{S28})$$

where $H(x)$ is a generating function defined as

$$H(x) = \sum_{k=0}^{\infty} Q(k+1)x^k, \quad (\text{S29})$$

and $Q(k) = kP(k)/\langle k \rangle$.

In Ref. [S5], the cavity method was used to calculate the controllability measure for directed networks with multiple types of self loops, where the diagonal elements of matrix L were regarded as self loops. This is key to calculating the locatability measure n_m for matrix $L - aI$. Adopting the method in Ref. [S5], we have that, if a diagonal element of $L - aI$ is nonzero, the in- and out-degree of the corresponding node is increased by 1, while the degrees of the other nodes remain the same in the original weighted network. For an undirected network, if a diagonal element of $L - aI$ is nonzero, the degree of the node is increased by 2. Finally, based on the new node degrees, we can obtain n_m by combining Eqs. (S25-S29).

V. Characteristics of real networks studied

In the main text, results from a number of real networks are presented to test our ET and FE methods. The details of the real networks are listed in table S1, which include the names of the data sets, the data type, the number of nodes N , the number of links E , and brief descriptions of the networks.

VI. Performance assessment of source localization

The area under a receiver operating characteristic (AUROC) for the source localization is defined in terms of true positive rate (TPR) and false positive rate (FPR). TPR and FPR are defined as follows:

$$\text{TPR}(s) = \frac{\text{TP}(s)}{P} \quad \text{and} \quad \text{FPR}(s) = \frac{\text{FP}(s)}{Q}, \quad (\text{S30})$$

where s is the cutoff (threshold) in the list of reconstructed state $x_i(t)$ at time t , $\text{TP}(s)$ ($\text{FP}(s)$) is the number of true (false) positives in the top s reconstructed values of $x_i(t)$ and P (Q) is the number of positives (negatives) in the gold standard. AUROC is the area under the TPR-FPR curve.

VII. More examples of source localization

A. An example of locating sources in undirected weighted ER network without noise

To be concrete, we set $\text{Data} = 0.5$ and assume that the initial triggering time t_0 is unknown. In Fig. S1A, we show that measurements from any single node are sufficient to locate the sources, as the network has a single connected component with random link weights. Fig. S1B shows that our method can accurately infer both the number of sources and their locations, as well as the initial triggering time t_0 . Fig. S1C shows, for different initial observation time t_{ini} , that the number of sources and their locations can be determined in a large range after t_0 is detected as in Fig. S1B.

The performance of our method can be assessed, as follows. For concreteness, we assume $t_{\text{ini}} = t_0 + 10$. Fig. S1D shows that the value of AUROC will reach unity at $t_{\text{ini}} - 10$, which is the triggering time t_0 , and the AUROC value decreases more significantly when the inferred time is $t < t_0$ as compared with the case of $t > t_0$. From Fig. S1E, we see that AUROC reaches unity when the observation time is $t_{\text{ini}} \approx 3$ time steps before t_0 , and AUROC is almost unchanged as t_{ini} is increased. These results are similar to those of SF networks (Fig. 3 in the main text).

B. Examples of locating sources in undirected weighted SF and ER networks in presence of noise

We extend our source localization framework to cases where there is noise for SF and ER networks. Assuming $\sigma = 0.5$ and setting $\text{Data} = 0.5$, we reconstruct $\mathbf{x}(t_0)$ with four random sources. Fig. S2 and Fig. S3 show essentially the same results as Fig. S1, indicating the robustness of our localization framework.

VIII. Robustness of our source localization framework

We systematically investigate source localization for undirected and weighted ER and SF networks in terms of data requirement and noise resistance. Supplementary Fig. S4A and Fig. S4B show, for $\sigma = 0$, relatively small data amount, and both ER and SF networks, that the value of AUROC increases when the number of sources is decreased. This means that the localization accuracy tends to increase with the sparsity of vector $\mathbf{x}(t_0)$. We also see that the value of AUROC exceeds 0.9 even though data amount is only 0.3, and unity value of AUROC can be achieved for $\text{Data} \geq 0.5$. For $\sigma = 0.5$, as shown in Supplementary Fig. S4C and Fig. S4D, similar results are obtained, except that the corresponding AUROC values are slightly smaller. As can be seen from Supplementary Fig. S4E and Fig. S4F, for $\text{Data} = 0.5$, the AUROC values are nearly indistinguishable for different values of N_s . For $\sigma \leq 0.3$, the value of AUROC reaches unity but will decrease with σ for $\sigma > 0.3$, regardless of the values of N_s . The AUROC reaches unity with error less than 5% despite that σ is as large as 0.5. All the results provide additional evidence for the robustness of our method against noise and insufficient data.

IX. Effects of diffusion parameter

We investigate the effects of the diffusion parameter β on the accuracy of source localization for different data amounts and values of the noise variance. In principle, to ensure that system (1) in the main text can characterize a diffusion process, the parameter β should be less than certain critical value. Specifically, we rewrite system (1) in the main text as

$$\begin{aligned} x_i(t+1) &= x_i(t) - \beta \sum_{j=1, j \neq i}^N w_{ji} x_i(t) + \beta \sum_{j=1, j \neq i}^N w_{ij} x_j(t), \\ &= \left(1 - \beta \sum_{j=1, j \neq i}^N w_{ji} \right) x_i(t) + \beta \sum_{j=1, j \neq i}^N w_{ij} x_j(t). \end{aligned} \quad (\text{S31})$$

Note that the coefficient of the first term on the right hand side of Eq.(S31) should be positive, for otherwise, the state $x_i(t+1)$ may become negative if $x_i(t)$ is large and positive and the value of the second term of Eq.(S31) is small. An example is shown in Fig. S5, where β is 0.15 and the coefficient $1 - \beta \sum_{j=1, j \neq i}^N w_{ji}$ associated with some nodes is negative. As a result, the state of a node, say $x_7(t)$, exhibits a negative value, causing the system to diverge. However, this scenario is not physically meaningful for describing a diffusion process. Thus, the following constraint on the coefficient $1 - \beta \sum_{j=1, j \neq i}^N w_{ji} > 0$ should be imposed:

$$\beta < \frac{1}{\sum_{j=1, j \neq i}^N w_{ji}}. \quad (\text{S32})$$

We find that, under the constraint, the choice of different values of β has little influence on the accuracy of source localization with respect to different data amounts and values of noise variance, as shown in Figs. S6 and S7. We see that, as β is decreased, e.g., $\beta = 0.01$, the localization accuracy is slightly reduced (Fig. S6), due to the computational errors associated with the iterative process in the implementation of the compressive sensing algorithm.

Supplementary Figures

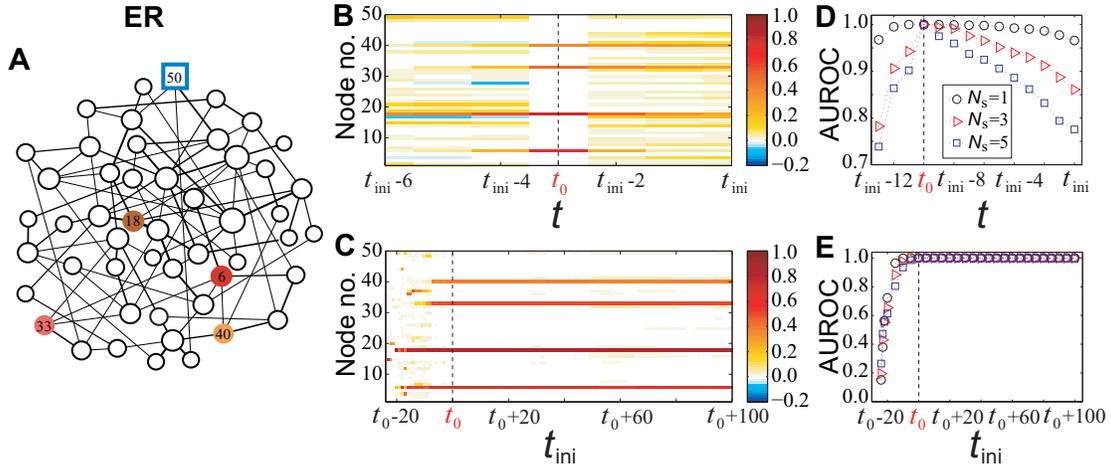


Fig. S1. An example of locating sources in undirected weighted ER networks. (A) Illustration of a ER network with four sources with colors representing the initial state values. One messenger node is specified as a blue square. The thickness of links represents their weight and the size of the nodes corresponds to their degrees. (B) Reconstructed state $x_i(t)$ of each node for $t \leq t_{ini}$, where the initial observation time is t_{ini} ($t_{ini} \geq t_0$). Colors represent the values of $x_i(t)$ with $t \leq t_{ini}$. (C) Reconstructed initial state $x_i(t_0)$ of each node from different initial observation time t_{ini} when t_0 , the true triggering time, is being successfully inferred. Colors represent the reconstructed values of $x_i(t_0)$. The colors have the same meanings as those in (A). The four sources are randomly selected and their $x_i(t_0)$ values are larger than zero. (D) AUROC as a function of t ($t \leq t_{ini}$) for a fixed initial observation time t_{ini} . (E) AUROC versus t for different initial observation time t_{ini} and different number of sources (N_s). For both (D) and (E), there is no noise, cases for different number of sources are illustrated, N_s , and t_0 is the true triggering time. In all cases, the network size is $N = 50$, the average degree is $\langle k \rangle = 4$, the link weights are uniformly distributed in $(0, 2)$, the diffusion parameter $\beta = 0.1$, and $Data = 0.5$. The results in (D) and (E) are obtained by averaging over 30 independent simulations. The other parameters are the same as in Fig. 5 in the main text.

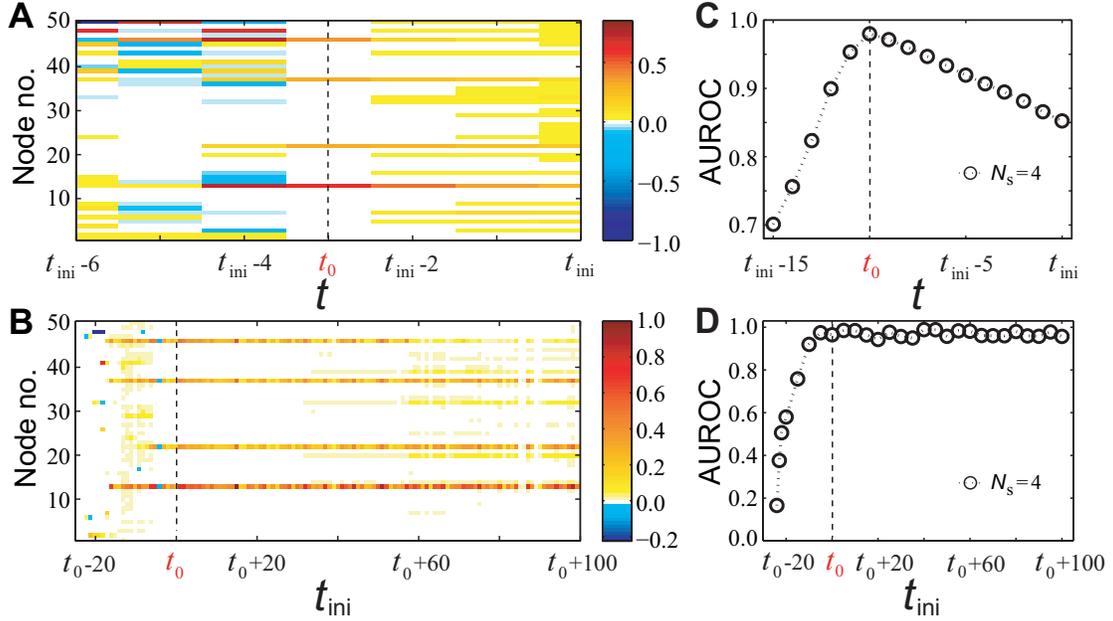


Fig. S2. An example of locating sources in undirected weighted SF network with noise. (A) Reconstructed state $x_i(t)$ of each node at time step t , for $t \leq t_{\text{ini}}$ and initial observation time t_{ini} ($t_{\text{ini}} \geq t_0$). (B) Reconstructed state $x_i(t)$ of each node for different initial observation time t_{ini} when t_0 is known. (C-D) AUROC as a function of (C) time t ($t \leq t_{\text{ini}}$) when the initial observation time is t_{ini} and as a function of (D) initial observation time t_{ini} . Network size is $N = 50$, the average degree is $\langle k \rangle = 4$, and the link weights are uniformly distributed in $(0, 2)$. Four sources are randomly selected and their initial states $x_i(t_0)$ assume positive values. We set $\beta = 0.05$, $\sigma = 0.5$, and $\text{Data} = 0.5$. The results in (C) and (D) are obtained by averaging over 30 independent simulations. The other parameters are the same as in Fig. 5 in the main text.

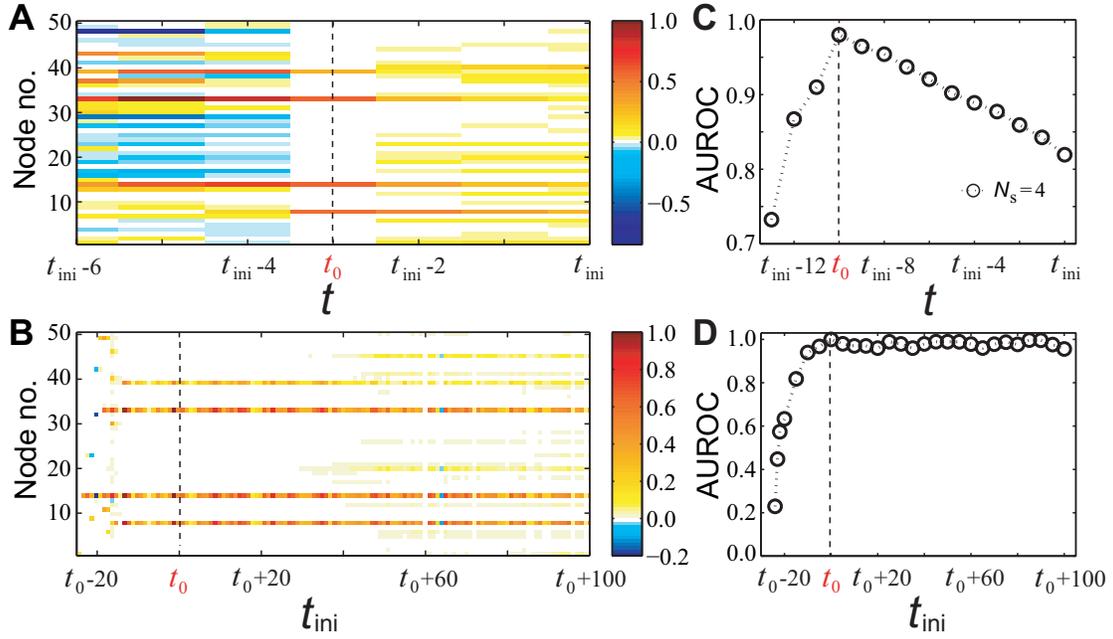


Fig. S3. An example of locating sources in undirected weighted ER network with noise. (A) Reconstructed state $x_i(t)$ of each node at time step t for $t \leq t_{\text{ini}}$ and for initial observation time t_{ini} ($t_{\text{ini}} \geq t_0$). (B) Reconstructed state $x_i(t)$ of each node for different initial observation time t_{ini} and for known t_0 . (C-D) AUROC as a function of (C) time t ($t \leq t_{\text{ini}}$) when the initial observation time is t_{ini} and as a function of (D) initial observation time t_{ini} . Network size is $N = 50$, the average degree is $\langle k \rangle = 4$, and the link weights are uniformly distributed in $(0, 2)$. Four sources are randomly selected and their initial state values $x_i(t_0)$ are positive. We set $\sigma = 0.5$, $\beta = 0.1$, and $\text{Data} = 0.5$. The results in (C) and (D) are obtained by averaging over 30 independent simulations. The other parameters are the same as in Fig. 5 in the main text.

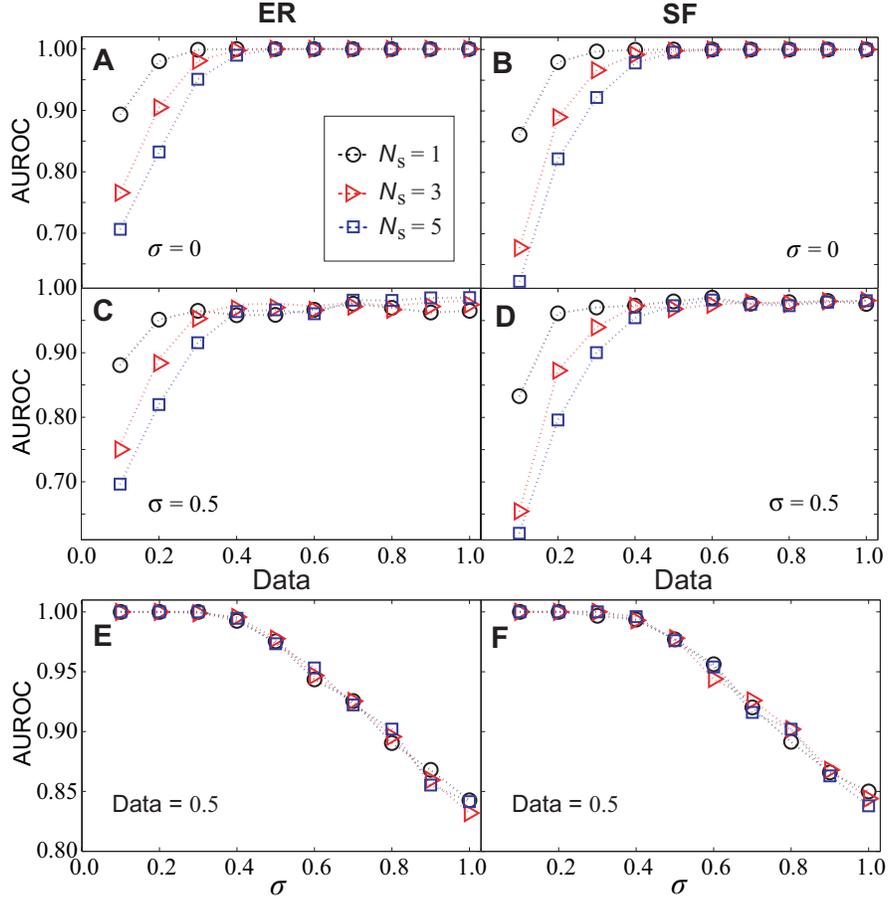


Fig. S4. Locating sources in weighted ER and SF networks. (A-B) In absence of noise, AUROC as a function of Data for different source number N_s for ER and SF networks, respectively. (C-D) The corresponding plots but with noise of amplitude $\sigma = 0.5$. (E-F) For Data = 0.5, AUROC as a function of σ for different values of N_s for ER and SF networks, respectively. The observational noise is modeled as $y(t)[1 + \mathcal{N}(0, \sigma^2)]$, where $\mathcal{N}(0, \sigma^2)$ is the Gaussian distribution. The baseline of AUROC is 0.5 (corresponding to random identification). The average degree is $\langle k \rangle = 4$ for both ER and SF networks and the link weights are uniformly distributed in $(0, 2)$. The network size is $N = 50$. We set $\beta = 0.1$ for ER networks and $\beta = 0.05$ for SF networks. The results are obtained by averaging over 1000 independent simulations. The other parameters are the same as in Fig. 5 in the main text.

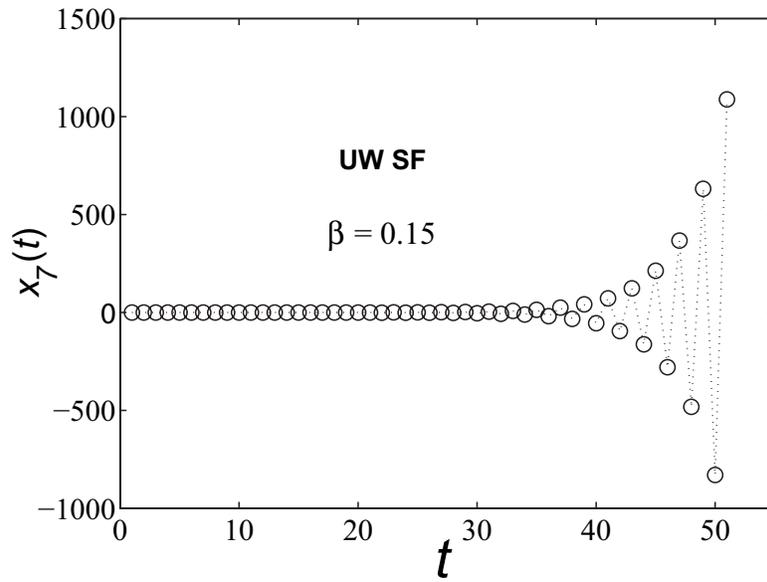


Fig. S5. Illustration of nodal state if the constraint on β is violated. The state $x_7(t)$ of node No. 7 as a function of time step t for $\beta = 0.15$ that violates the constraint on β (Eq. (S32)). $x_7(t)$ presents negative value and tends to diverge as t increases. The degree k_i of node No. 7 is 10, the average degree $\langle k \rangle$ of the unweighted SF network is 4 and the network size N is 50. The number of sources N_s is 3.

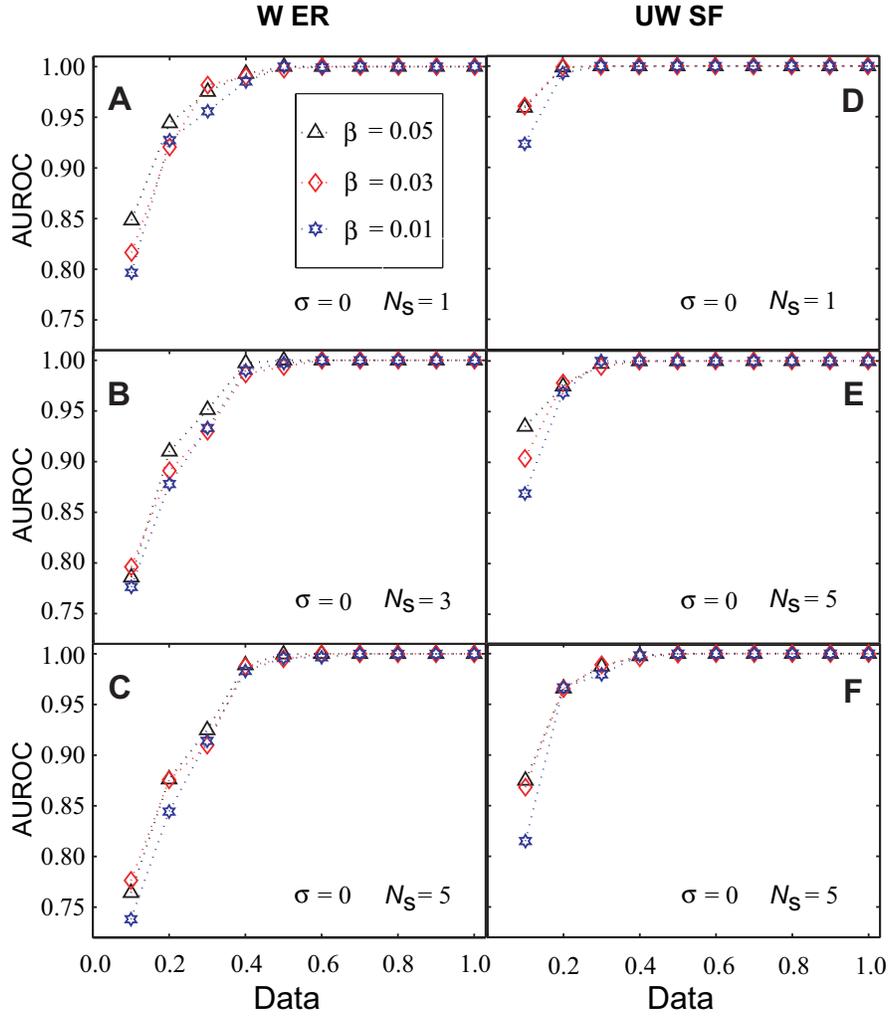


Fig. S6. Effect of β on source localization in networks from different amounts of data. (A-F) AUROC as a function of Data for different number N_S of sources for (A-C) weighted ER networks and (D-F) for unweighted SF networks, respectively. For ER networks, $\langle k \rangle = 2$ and for SF networks $\langle k \rangle = 4$. For weighted networks, the link weights are randomly selected from an uniform distribution in the range $(0, 2)$. The network size N is 50 and noise variance $\sigma = 0$. The results are obtained by averaging over 100 independent simulations. The other parameters are the same as in Fig. 5 in the main text.

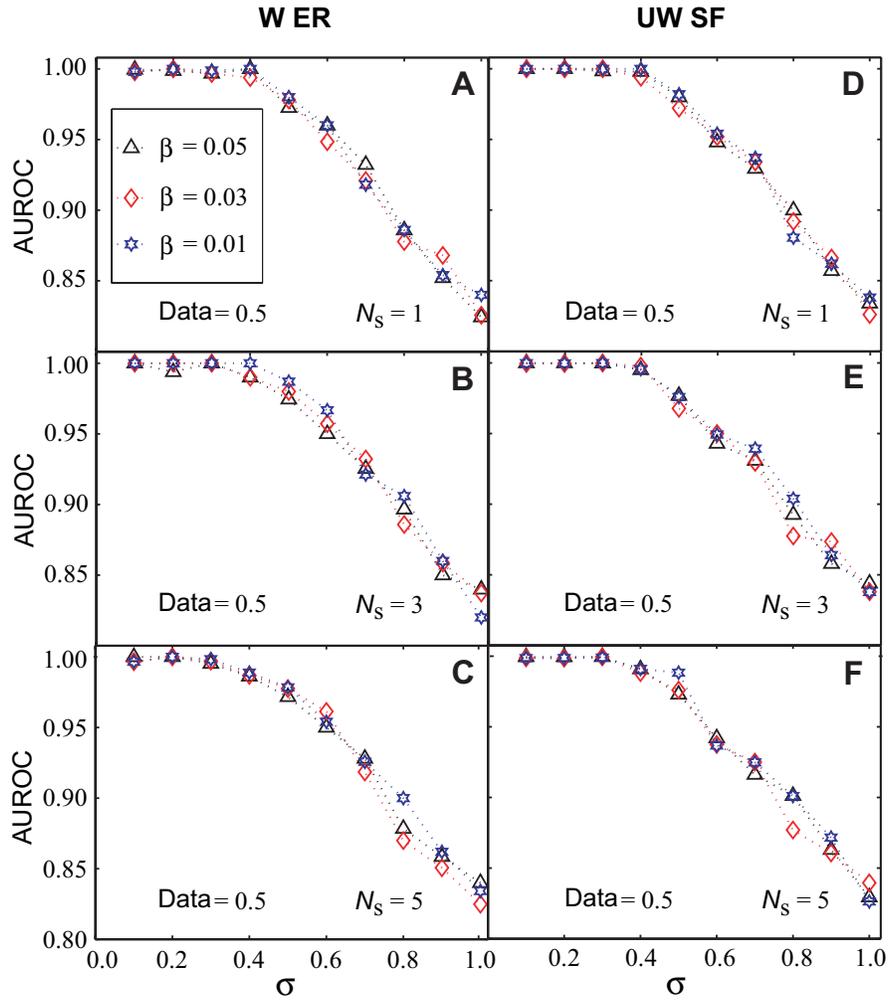


Fig. S7. Effect of β on source localization in networks from noisy data. (A-F) AUROC as a function of noise variance σ for (A-C) weighted ER and (D-F) unweighted SF networks, respectively. The white Gaussian noise is in the form $y(t)[1 + \mathcal{N}(0, \sigma^2)]$, where $\mathcal{N}(0, \sigma^2)$ is the Gaussian distribution. Data = 0.5 and the results are obtained by averaging over 300 independent simulations. The other parameters are the same as in fig. S6.

Supplementary Table

Table S1. Summary of the real networks used in Fig. 3 in the main text. The quantities N and E denote the network size and the number of links, respectively. UD (D) in the Type column indicates undirected (directed) networks. The structural data of all the networks are available online. The data of Erdős971 can be downloaded via <http://vlado.fmf.uni-lj.si/pub/networks/pajek/data/gphs.htm>, and the data of USAir can be downloaded via <http://vlado.fmf.uni-lj.si/pub/networks/data/map/USAir97.net>.

Data sets Name	Type	N	E	Description
ca-GrQc [S7]	UD	5242	14496	collaboration network of Arxiv General Relativity category
ca-HepTh [S7]	UD	9877	25598	collaboration network of Arxiv High Energy Physics Theory category
Erdős971	UD	433	1314	all of Paul Erdős's coauthors and their respective coauthors
dolphin [S8]	UD	62	159	associations between dolphins in a community living off Doubtful Sound
football [S9]	UD	115	613	American football games between Division IA colleges during regular season Fall 2000
Jazz [S10]	UD	198	2742	links of the network of Jazz musicians
Zachary's karate club [S11]	UD	34	78	social network of friendships of a karate club at a US university in the 1970s
Political blogs [S12]	D	1224	19025	hyperlinks between weblogs on US politics in 2005 by Adamic and Glance
Wiki-Vote [S13, 14]	D	7115	103689	all the Wikipedia voting data from the inception of Wikipedia till January 2008
E-mail [S15]	UD	1133	5451	interchanges between members of the Univeristy Rovira i Virgili (Tarragona)
p2p-Gnutella [S16]	D	6301	20777	Gnutella peer-to-peer network on August 8 2002
PGP [S17]	UD	10680	24236	links of the giant component of the network of users of the Pretty-Good-Privacy algorithm for secure information interchange
USAir	UD	332	2126	US Air flights, 1997

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