Measuring the importance of individual units in producing the collective behavior of a complex network

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Abstract

A quantitative evaluation of the contribution of individual units in producing the collective behavior of a complex network can allow us to understand the potential damage to the structure integrity due to the failure of local nodes. Given time series for the units, a natural way to do this is to find the information flowing from the unit of concern to the rest of the network. In this study, we show that this flow can be rigorously derived in the setting of a continuous-time dynamical system. With a linear assumption, a maximum likelihood estimator can be obtained, allowing us to estimate it in an easy way. As expected, this “cumulative information flow” does not equal to the sum of the information flows to other individual units, reflecting the collective phenomenon that a group is not the addition of the individual members. For the purpose of demonstration and validation, we have examined a network made of Stuart-Landau oscillators. Depending on the topology, the computed information flow may differ. In some situations, the most crucial nodes for the network are not the hubs; they may have low degrees, and, if depressed or attacked, will cause the failure of the entire network.

Keywords: Information flow, causality, complex networks, collective behavior, network robustness.

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I. INTRODUCTION

Complex networks provide a framework for the studies of many social, biological, and engineering systems such as the internet, brains, power grids, financial trading markets, food webs, gene regulatory networks, to name a few. A network consists of nodes or vertexes standing for the individual units or organizations, and links or edges for the interactions among the nodes. For a node, the number of links connected to other nodes is called its degree. By degree distribution we can have homogeneous and heterogeneous networks. The former class has binomial or Poisson degree distributions, examples including random graphs\[1\] and small-world networks\[2\], while the latter class is scale free, bearing probability distributions $P$ of degree $k$ following a power law $P(k) \sim k^{-\gamma}$, with an exponent $\gamma \sim 2 - 3$. Most social\[3\], biological\[4\], and technological networks\[5\] have the scale-free property; other topological properties include high clustering coefficient, community and hierarchical structures, and, for directed networks, reciprocity, triad significance profile, etc.

A goal of complex network studies is to understand how individuals collaborate to produce the collective behavior. One question to ask is whether the connectivity of a network is robust to local node failure, deterioration or functional depression. Of particular interest is whether initially a tiny shock may cascade to disrupt the network on a large scale. How to quantify the contribution of a unit to the network as a whole is hence an important issue; it is related to many real world problems such as power grid failure (e.g., the 2003 massive blackout that darkened much of the North American upper Midwest and Northeast\[6\]), control of epidemic disease, identification of bottlenecks in city traffic, etc. Usually this is studied by observing the connectivity after preferential removal of a unit, which is found to have different effects on the two types of networks. If the removal or attack is random, heterogeneous networks are quite robust as compared to homogeneous networks; if, however, the attack is intentional at some special nodes, then heterogeneous networks could be rather fragile. These special nodes are usually highly connected ones, i.e., hubs, as easily imagined. Recently, Tanaka et al.\[7\] observed that, sparsely connected nodes may be more important which, if functionally depressed, may result in drastic change in network structure. That is to say, the structure integrity or robustness could also be largely influenced by low-degree nodes, rather than by hubs. We hence cannot judge the importance of a unit simply by degree. It depends on many different properties of the network topology in question.
As said above, the problem is usually tackled by removing a unit and observing the change in topology of the network of concern. However, in many networks, biological networks in particular, this is often infeasible, as breaking a unit means terminating the experiment. On the other hand, we may have time series of measurements. So the whole problem is converted into assessing the importance of a unit from analyzing the signals as observed. Previously, we have rigorously formulated information flow within dynamical systems (e.g., [8][9]); it has been widely used for studying the causal relations among dynamical events, and hence is readily for the study of the interactions among nodes in a network. One may think that the contribution of a given node may be obtained by adding up all the information flows from it to the other nodes. Unfortunately, as we will see soon in the following sections, this is true only when all the nodes are disconnected, i.e., when the nodes do not form a network and hence no collective behavior emerge. This from one aspect manifests the well-known fact that groups are not simply the addition of their individual members; they could be more or less (some social science examples can be seen in [10][11][12][13]).

In the following, we first present the setting for the problem, and then derive the information flow from an individual unit to the network. Maximum likelihood estimation is made in section III; it yields a formula for easy assessment of the importance of a node from given time series. As a validation, and also a demonstration of application, section IV presents a network of synchronized Stuart-Landau oscillators which, when a fraction of nodes become deteriorated, may become silent completely. This study is concluded in section V.

II. INFORMATION FLOW FROM A UNIT TO THE ENTIRE NETWORK

Consider a network modeled by an \( n \)-dimensional dynamical system

\[
\frac{dx}{dt} = F(x, t) + B(x, t)\dot{w},
\]

where \( x \) is the state variable vector for the \( n \) nodes \((x_1, x_2, \ldots, x_n)\), \( x \in \mathbb{R}^n \), \( F = (F_1, \ldots, F_n) \) the differentiable functions of \( x \) and time \( t \) describe the interaction paths (edges/links), \( w \) is a vector of \( m \) independent standard Wiener processes, and \( B = (b_{ij}) \) an \( n \times m \) is the matrix of stochastic perturbation amplitude. Here we follow the convention in physics not to distinguish a random variable and a deterministic variable. (In probability theory, they are usually distinguished
by upper-case and low-case symbols.) To examine the influence of a unit to the entire network made of the $n$ units, it suffices to consider the component $x_1$; if not, we can always re-arrange the vector $x$ to make it so. The whole problem now boils down to finding the information flow from $x_1$ to $(x_2, x_3, ..., x_n)$, which we will be denoting as $x_{2..n}$ henceforth (i.e., as $x$ with component 1 removed).

In [9], the information flow between two individual components $x_i$ and $x_j$ has been rigorously derived from first principles. But the information flow from one component, here $x_1$, to a multitude of components, here $x_{2..n}$, is yet to be implemented. One may conjecture that it is just an addition of all flows from $x_1$ to all the individual components of $x_{2..n}$. As we will see soon below, this is generally not the case, and the nonadditivity is a reflection of the macrostate or collective behavior of a multi-connected network.

We follow the strategy used in [15] to do the derivation. The information flow is, by the physical argument therein, the amount of entropy transferred from $x_1$ to $x_{2..n}$. We hence need to find the evolution of the joint entropy of $x_{2..n}$, and single out the contribution to this evolution from $x_1$. This result follows.

**Theorem II.1** For the dynamical system (1), if the probability density function (pdf) of $x$ is compactly supported, then the information flow from $x_1$ to $(x_2, x_3, ..., x_n)$ is

$$T_{1\rightarrow2..n} = -E \left[ \sum_{i=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial F_i}{\partial x_i} \rho_{2..n} \right] + \frac{1}{2} E \left[ \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial^2 g_{ij}}{\partial x_i \partial x_j} \rho_{2..n} \right].$$

(2)

The units are nats per unit time. In the equation, $\rho_{2..n}$ is joint pdf of $(x_2, x_3, ..., x_n)$, $g_{ij} = \sum_{k=1}^{n} b_{ik}b_{jk}$, and $E$ signifies mathematical expectation.

**Proof.** Associated with (1) there is a Fokker-Planck equation governing the evolution of the pdf $\rho$ of $x$:

$$\frac{\partial \rho}{\partial t} + \frac{\partial F_1}{\partial x_1} + \frac{\partial F_2}{\partial x_2} + ... + \frac{\partial F_n}{\partial x_n} = \frac{1}{2} \sum_{i=1}^{d} \sum_{j=1}^{n} \frac{\partial^2 g_{ij}}{\partial x_i \partial x_j} \rho,$$

(3)

where $g_{ij} = \sum_{k=1}^{n} b_{ik}b_{jk}$, $i, j = 1, ..., n$. This marginal pdf of $x_1$, $\rho_1(x_1)$, is obtained by integrating out $(x_2, ..., x_n)$ in (3). By the assumption of compactness of $\rho$, the resulting equation becomes

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial}{\partial x_1} \int_{\mathbb{R}^{n-1}} \rho F_1 d\mathbf{x}_{2..n} = \frac{1}{2} \frac{\partial^2}{\partial x_1^2} \int_{\mathbb{R}^{n-1}} g_{11} \rho d\mathbf{x}_{2..n}.$$
For the sake of notational simplicity, here we have written \( dx_2dx_3...dx_n \) as \( d\mathbf{x}_{2..n} \). From this the evolution of the marginal entropy of \( x_1 \), written \( H_1 \), can be derived:

\[
\frac{dH_1}{dt} = -E \left[ F_1 \frac{\partial \log \rho_1}{\partial x_1} \right] - \frac{1}{2} E \left[ g_{11} \frac{\partial \log \rho_1}{\partial x_2} \right].
\] (5)

See Liang (2008) for a proof.

To study impact of \( x_1 \) on the rest of the network, we need to consider the evolution of the joint entropy of \( (x_2, x_3, ... x_n) = \mathbf{x}_{2..n} \), i.e.,

\[
H_{2..n} = -\int_{\mathbb{R}^{n-1}} \rho_{2..n} \log \rho_{2..n} d\mathbf{x}_{2..n},
\]

where \( \rho_{2..n} = \rho_{2..n}(x_2, ..., x_n) = \int_{\mathbb{R}} \rho dx_1 \) is the joint pdf of \( (x_2, x_3, ... x_n) \).

By integrating out \( x_1 \) from Eq. 3, we have

\[
\frac{\partial \rho_{2..n}}{\partial t} + \frac{\partial}{\partial x_2} \int_{\mathbb{R}} \rho F_1 dx_1 + \ldots + \frac{\partial}{\partial x_n} \int_{\mathbb{R}} \rho F_n dx_1 = \frac{1}{2} \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{\partial^2}{\partial x_i \partial x_j} \int_{\mathbb{R}} g_{ij} \rho dx_1.
\] (6)

Multiply \(-1 + \log \rho_{2..n}\), then integrate over \( \mathbb{R}^{n-1} \). The first term is \( dH_{2..n}/dt \). By taking advantage of the compactness assumption, the second term on the left hand side results in

\[
- \int_{\mathbb{R}^{n-1}} \left[ (1 + \log \rho_{2..n}) \frac{\partial}{\partial x_2} \left( \int_{\mathbb{R}} \rho F_2 dx_1 \right) \right] d\mathbf{x}_{2..n}
\]

\[
= - \int_{\mathbb{R}^{n-1}} \log \rho_{2..n} \frac{\partial}{\partial x_2} \left( \int_{\mathbb{R}} \rho F_2 dx_1 \right) d\mathbf{x}_{2..n}
\]

\[
= \int_{\mathbb{R}^{n-2}} \left\{ \left[ -\log \rho_{2..n} \cdot \int_{\mathbb{R}} \rho F_2 dx_1 \right] - \int_{\mathbb{R}} \left( \int_{\mathbb{R}} \rho F_2 dx_1 \right) \frac{\partial \log \rho_{2..n}}{\partial x_2} dx_2 \right\} dx_3...dx_n
\]

\[
= \int_{\mathbb{R}^n} \rho F_2 \frac{\partial \log \rho_{2..n}}{\partial x_2} dx = E \left[ F_2 \frac{\partial \log \rho_{2..n}}{\partial x_2} \right],
\]

where \( E \) signifies mathematical expectation. Likewise, the third term through the \( n^{th} \) term are

\[
E \left[ F_3 \frac{\partial \log \rho_{2..n}}{\partial x_3} \right], \ldots, E \left[ F_n \frac{\partial \log \rho_{2..n}}{\partial x_n} \right].
\]
On the right hand side, the \((i, j)^{th}\) component is

\[
- \int_{\mathbb{R}^{n-1}} \left[ (1 + \log \rho_{2..n}) \cdot \frac{1}{2} \frac{\partial^2}{\partial x_i \partial x_j} \int_{\mathbb{R}} g_{ij} \rho dx_1 \right] dx_{2..n}
\]

\[
= - \frac{1}{2} \int_{\mathbb{R}^{n-1}} \log \rho_{2..n} \cdot \frac{\partial^2}{\partial x_i \partial x_j} \left( \int_{\mathbb{R}} g_{ij} \rho dx_1 \right) dx_{2..n}
\]

\[
= - \frac{1}{2} \int_{\mathbb{R}^{n-2}} \left\{ \left[ \log \rho_{2..n} \cdot \frac{\partial}{\partial x_j} \left( \int_{\mathbb{R}} g_{ij} \rho dx_1 \right) \right]_{-\infty}^{\infty} \right.
\]

\[
- \int_{\mathbb{R}} \frac{\partial \log \rho_{2..n}}{\partial x_i} \cdot \frac{\partial}{\partial x_j} g_{ij} \rho dx_1 \right\} dx_2...dx_i+1...dx_n
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^{n-1}} \frac{\partial \log \rho_{2..n}}{\partial x_i} \cdot \frac{\partial}{\partial x_j} g_{ij} \rho dx_1 \right\} dx_{2..n}
\]

\[
= \frac{1}{2} \int_{\mathbb{R}^{n-2}} \left\{ \left[ \frac{\partial \log \rho_{2..n}}{\partial x_i} \int_{\mathbb{R}} g_{ij} \rho dx_1 \right]_{-\infty}^{\infty} \right.
\]

\[
- \int_{\mathbb{R}} \left( \int_{\mathbb{R}} g_{ij} \rho dx_1 \right) \cdot \frac{\partial^2 \log \rho_{2..n}}{\partial x_i \partial x_j} dx_1 \right\} dx_2...dx_j-1dx_j+1...dx_n
\]

\[
= - \frac{1}{2} \int_{\mathbb{R}^n} \rho g_{ij} \frac{\partial^2 \log \rho_{2..n}}{\partial x_i \partial x_j} dx = - \frac{1}{2} \mathbb{E} \left[ g_{ij} \frac{\partial^2 \log \rho_{2..n}}{\partial x_i \partial x_j} \right].
\]

Putting the above together, we have

\[
\frac{dH_{2..n}}{dt} = - \sum_{i=2}^{n} \mathbb{E} \left[ F_i \frac{\partial \log \rho_{2..n}}{\partial x_i} \right] - \frac{1}{2} \sum_{i=2}^{n} \sum_{j=2}^{n} \mathbb{E} \left[ g_{ij} \frac{\partial^2 \log \rho_{2..n}}{\partial x_i \partial x_j} \right]. \quad (7)
\]

The evolution of \(H_{2..n}\) contains two parts, one being the effect of \(x_1\), another being the part with the effect of \(x_1\) excluded. We denote the latter by \(dH_{2..n,1}/dt\); it can be found by instantaneously freezing \(x_1\) as a parameter. For this purpose, we examine, on an infinitesimal interval \([t, t+\Delta t]\), a system modified from the original (1) by removing its first equation, i.e.,

\[
\frac{dx_2}{dt} = F_2(x_1, x_2, ..., x_n; t) + \sum_{k=1}^{m} b_{2k}(x_1, x_2, ..., x_n; t) \tilde{w}_k \quad (8)
\]

\[
\frac{dx_3}{dt} = F_3(x_1, x_2, ..., x_n; t) + \sum_{k=1}^{m} b_{3k}(x_1, x_2, ..., x_n; t) \tilde{w}_k \quad (9)
\]

\[
\vdots
\]

\[
\frac{dx_n}{dt} = F_n(x_1, x_2, ..., x_n; t) + \sum_{k=1}^{m} b_{nk}(x_1, x_2, ..., x_n; t) \tilde{w}_k. \quad (10)
\]
Note here the $F_i$’s and $b_{ik}$’s still have dependence on $x_1$, but now $x_1$ appears in the modified system as a parameter. Given the pdf of $x$ at time $t$, we need to find the pdf of $x_1$ at time $t + \Delta t$. In Liang (2016), this is fulfilled by first constructing a mapping $\Phi : \mathbb{R}^{n-1} \to \mathbb{R}^{n-1}$, $x_1(t) \mapsto x_1(t + \Delta t)$, then studying the Frobenius-Perron operator of the modified system. Here we choose an alternative approach. Note on the interval $[t, t + \Delta t]$, there also exists a Fokker-Planck equation for the modified system

$$\frac{\partial \rho_1}{\partial t} + \frac{\partial F_2 \rho_1}{\partial x_2} + \frac{\partial F_3 \rho_1}{\partial x_3} + \ldots + \frac{\partial F_n \rho_1}{\partial x_n} = \frac{1}{2} \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{\partial^2 g_{ij} \rho_1}{\partial x_i \partial x_j},$$ (11) 

$$\rho_1 = \rho_{2..n} \quad \text{at time } t.$$ (12)

Here $g_{ij} = \sum_{k=1}^{m} b_{ik} b_{jk}$ is still as before; $\rho_1$ means the joint pdf of $(x_2, \ldots, x_n)$ with $x_1$ frozen as a parameter. $\rho_1$ is somehow similar to the conditional pdf of the former on the latter, but not exactly as that. The subscript $\backslash 1$ signifies that $x_1$ is removed from the independent variables. Note this is quite different from $\rho_{2..n}$, which has no dependence on $x_1$ at all; but they are equal at time $t$.

Divide (11) by $\rho_1$ to get

$$\frac{\partial \log \rho_1}{\partial t} + \sum_{i=2}^{n} \frac{1}{\rho_1} \frac{\partial F_i \rho_1}{\partial x_i} = \frac{1}{2} \rho_1 \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{\partial^2 g_{ij} \rho_1}{\partial x_i \partial x_j}.$$

Discretizing, and noticing that $\rho(t) = \rho_{2..n}(t)$, we have

$$\log \rho(x_1; t + \Delta t) = \log \rho_{2..n}(x_1; t) - \Delta t \cdot \sum_{i=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial F_i \rho_{2..n}}{\partial x_i} + \frac{\Delta t}{2} \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial^2 g_{ij} \rho_{2..n}}{\partial x_i \partial x_j} + o(\Delta t).$$

To arrive $dH_{2..n, \backslash 1}/dt$, we need to find $\log \rho(x_1(t + \Delta t); t + \Delta t)$. Using the Euler-Bernstein approximation,

$$x_1(t + \Delta t) = x_1(t) + F_1 \Delta t + B_1 \Delta w,$$ (13)

where, just like the notation $x_1$,

$$F_1 = (F_2, \ldots, F_n)^T,$$

$$B_1 = \begin{bmatrix} b_{21} & \ldots & b_{2m} \\ \vdots & \ddots & \vdots \\ b_{n1} & \ldots & b_{nm} \end{bmatrix}$$

$$\Delta w = (\Delta w_1, \ldots, \Delta w_m)^T$$
and $\Delta w_k \sim N(0, \Delta t)$, we have

$$
\log(\rho_i(x(t + \Delta t); t + \Delta t)) = \log \rho_{2,n}(x(t) + F_1 \Delta t + B_1 \Delta w; t)
$$

$$
= -\Delta t \cdot \sum_{i=2}^{n} \frac{1}{\rho_{2,n}} \frac{\partial F_i \rho_{2,n}}{\partial x_i} + \Delta t \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{1}{\rho_{2,n}} \frac{\partial^2 g_{ij} \rho_{2,n}}{\partial x_i \partial x_j} + o(\Delta t).
$$

$$
+ \frac{1}{2} \cdot \sum_{i=2}^{n} \sum_{j=2}^{n} \left[ \frac{\partial^2 \log \rho_{2,n}(F_i \Delta t + \sum_{k=1}^{m} b_{ik} \Delta w_k)(F_j \Delta t + \sum_{l=1}^{m} b_{jl} \Delta w_l)}{\partial x_i \partial x_j} \right]
$$

$$
- \Delta t \cdot \sum_{i=2}^{n} \frac{1}{\rho_{2,n}} \frac{\partial F_i \rho_{2,n}}{\partial x_i} + \Delta t \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{1}{\rho_{2,n}} \frac{\partial^2 g_{ij} \rho_{2,n}}{\partial x_i \partial x_j} + o(\Delta t).
$$

Take mathematical expectation on both sides. The left hand side is $-H_{2,n}(t + \Delta t)$. By the Corollary III.1 of Liang (2016), and noting $E\Delta w_k = 0$, $E\Delta w_k^2 = \Delta t$ and the fact that $\Delta w$ are independent of $x_1$, we have

$$
-H_{2,n}(t + \Delta t) = -H_{2,n}(t) + \Delta t \cdot E \sum_{i=2}^{n} F_i \frac{\partial \log \rho_{2,n}}{\partial x_i}
$$

$$
+ \frac{\Delta t}{2} \cdot E \sum_{i=2}^{n} \sum_{j=2}^{n} \sum_{k=1}^{m} \sum_{l=1}^{m} b_{ik} b_{jl} \delta_{kl} \frac{\partial^2 \log \rho_{2,n}}{\partial x_i \partial x_j}
$$

$$
- \Delta t \cdot E \sum_{i=2}^{n} \frac{1}{\rho_{2,n}} \frac{\partial F_i \rho_{2,n}}{\partial x_i} + \Delta t \cdot E \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{1}{\rho_{2,n}} \frac{\partial^2 g_{ij} \rho_{2,n}}{\partial x_i \partial x_j} + o(\Delta t)
$$

$$
= -H_{2,n}(t) + \Delta t \cdot E \sum_{i=2}^{n} F_i \frac{\partial \log \rho_{2,n}}{\partial x_i} + \frac{\Delta t}{2} \cdot E \sum_{i=2}^{n} \sum_{j=2}^{n} g_{ij} \frac{\partial^2 \log \rho_{2,n}}{\partial x_i \partial x_j}
$$

$$
- \Delta t \cdot E \sum_{i=2}^{n} \frac{1}{\rho_{2,n}} \frac{\partial F_i \rho_{2,n}}{\partial x_i} + \frac{\Delta t}{2} \cdot E \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{1}{\rho_{2,n}} \frac{\partial^2 g_{ij} \rho_{2,n}}{\partial x_i \partial x_j} + o(\Delta t).
$$

So

$$
\frac{dH_{2,n}(t)}{dt} = \lim_{\Delta t \to 0} \frac{H_{2,n}(t + \Delta t) - H_{2,n}(t)}{\Delta t}
$$

$$
= -E \sum_{i=2}^{n} \left( F_i \frac{\partial \log \rho_{2,n}}{\partial x_i} - \frac{1}{\rho_{2,n}} \frac{\partial F_i \rho_{2,n}}{\partial x_i} \right)
$$

$$
- \frac{1}{2} E \sum_{i=2}^{n} \sum_{j=2}^{n} \left( g_{ij} \frac{\partial^2 \log \rho_{2,n}}{\partial x_i \partial x_j} + \frac{1}{\rho_{2,n}} \frac{\partial^2 g_{ij} \rho_{2,n}}{\partial x_i \partial x_j} \right).
$$
Hence the information flow from $x_1$ to $x_1$ is

$$T_{1\to2..n} = \frac{dH_{2..n}}{dt} - \frac{dH_{2..n,\lambda}}{dt}$$

$$= -E \sum_{i=2}^{n} \left( F_i \frac{\partial \log \rho_{2..n}}{\partial x_i} \right) - \frac{1}{2} E \sum_{i=2}^{n} \sum_{j=2}^{n} \left( g_{ij} \frac{\partial^2 \log \rho_{2..n}}{\partial x_i \partial x_j} \right)$$

$$- E \sum_{i=2}^{n} \frac{\partial F_i}{\partial x_i} + \frac{1}{2} E \sum_{i=2}^{n} \sum_{j=2}^{n} \left( g_{ij} \frac{\partial^2 \log \rho_{2..n}}{\partial x_i \partial x_j} + \frac{1}{\rho_{2..n}} \frac{\partial^2 g_{ij} \rho_{2..n}}{\partial x_i \partial x_j} \right)$$

$$= -E \left[ \sum_{i=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial F_i \rho_{2..n}}{\partial x_i} \right] + \frac{1}{2} E \left[ \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial^2 g_{ij} \rho_{2..n}}{\partial x_i \partial x_j} \right].$$

Q.E.D.

There is a nice property regarding noise: when the noise is additive, the stochastic contribution to the information flow vanishes, as stated in the following corollary.

**Corollary 1** In (1), if $B_1$ does not depend on $x$, then

$$T_{1\to2..n} = -E \left[ \sum_{i=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial F_i \rho_{2..n}}{\partial x_i} \right].$$

**Proof.** If $b_{ij}$ is independent of $x$, so is $g_{ij} = \sum_{k=1}^{n} b_{ik} b_{jk}$. Thus,

$$E \sum_{i} \sum_{j} \frac{1}{\rho_{2..n}} \frac{\partial^2 g_{ij} \rho_{2..n}}{\partial x_i \partial x_j} = \sum_{i} \sum_{j} g_{ij} \int_{R^n} \frac{\partial^2 \rho_{2..n}}{\partial x_i \partial x_j} dx$$

$$= \sum_{i} \sum_{j} g_{ij} \int_{R^{n-1}} \rho dx_1 \frac{\partial^2 \rho_{2..n}}{\partial x_i \partial x_j} dx_2 dx_3...dx_n$$

$$= \sum_{i} \sum_{j} g_{ij} \int_{R^{n-1}} \frac{\partial^2 \rho_{2..n}}{\partial x_i \partial x_j} dx_2 dx_3...dx_n,$$

which is zero by the compactness of $\rho$. Q.E.D.

The formula (2) can be verified with the particular situation in which the rest of the network does not depend on $x_1$. In this case $x_1$ plays no role. Indeed, if we follow the procedure for the above corollary, it is easy to prove that $T_{1\to2..n}$ vanishes. So we have:

**Theorem II.2** (Principle of nil causality) If $F_1$ and $B_1$ are independent of $x_1$, $T_{1\to2..n} = 0$. 

9
A. Linear systems

Steered by a linear system, a Gaussian process is always Gaussian. In this case, the information flow can be greatly simplified.

Theorem II.3 In (1), suppose

\[ F_i = f_i + \sum_{j=1}^{n} a_{ij} x_j, \]  

(14)

where \( f_i \) and \( a_{ij} \) are constants, and \( b_{ij} \) are also constants. Further suppose that initially \( x \) has a Gaussian distribution, then

\[ T_{1\to 2..n} = \sum_{i=2}^{n} \left[ \sum_{j=2}^{n} \sigma'_{ij} \left( \sum_{k=1}^{n} a_{ik} \sigma_{kj} \right) - a_{ii} \right], \]

(15)

where \( \sigma'_{ij} \) is the \((i, j)\)th entry of

\[
\begin{bmatrix}
1 & 0 \\
0 & \Sigma^{-1}
\end{bmatrix}
\]

Proof. In (2), by Corollary 1, the stochastic part (second term) can be ignored. Suppose the joint pdf of \( x \) has a form like

\[ \rho(x_1, \ldots, x_n) = \frac{1}{\sqrt{(2\pi)^n \det \Sigma}} e^{-\frac{1}{2}(x-\mu)^T \Sigma^{-1} (x-\mu)}. \]

(16)

Then it is easy to show

\[ \rho_{2..n}(x_2, \ldots, x_n) = \frac{1}{\sqrt{(2\pi)^{n-1} \det \Sigma\_1}} e^{-\frac{1}{2}(x_1-\mu_1)^T \Sigma\_1^{-1} (x_1-\mu_1)}, \]

(17)

where \( \Sigma\_1 \) is the covariance matrix \( \Sigma \) with the first row and first column deleted, and \( \mu_1 \) is the vector \( \mu \) with the first entry removed. For easy correspondence, we will still count the entries as those as numbered in \( \Sigma \) and \( \mu \). So

\[
F_i \frac{\partial \log \rho_{2..n}}{\partial x_i} \left[ f_i + \sum_{j=1}^{n} a_{ij} x_j \right] \frac{\partial}{\partial x_i} \left[ -\frac{1}{2} (x_q - \mu_q)^T \Sigma_q^{-1} (x_q - \mu_q) \right]
\]

\[ = \left( f_i + \sum_{j=1}^{n} a_{ij} x_j \right) \sum_{j=2}^{n} \left( -\frac{\sigma'_{ij} + \sigma'_{ji}}{2} \right) (x_j - \mu_j). \]
Here $\sigma'_{ij}$ is the $(i, j)^{th}$ entry of the matrix $\Sigma^{-1}_{q}$. (Note here the entry indices run from 2 through $n$, not from 1 through $n$!) As $\Sigma_{q}$ is symmetric, so is $\Sigma^{-1}_{q}$, and hence $(\sigma'_{ij} + \sigma'_{ji})/2 = \sigma'_{ij}$. So

$$-EF_{i} \frac{\partial \log \rho_{2..n}}{\partial x_{i}} = 0 - E \sum_{j=1}^{n} a_{ij} x_{j} \cdot \sum_{j=2}^{n} (-\sigma'_{ij}) \cdot (x_{j} - \mu_{j})$$

$$= E \sum_{k=1}^{n} a_{ik} (x_{k} - \mu_{k}) \cdot \sum_{j=2}^{n} \sigma'_{ij} (x_{j} - \mu_{j})$$

$$= \sum_{k=1}^{n} \sum_{j=2}^{n} a_{ik} \sigma'_{ij} E (x_{k} - \mu_{k}) (x_{j} - \mu_{j})$$

$$= \sum_{k=1}^{n} \sum_{j=2}^{n} a_{ik} \sigma'_{ij} \sigma_{k.j}.$$  

The other term

$$-E \sum_{i=2}^{n} \frac{\partial F_{i}}{\partial x_{i}} = - \sum_{i=2}^{n} a_{ii}.$$  

Eq. (15) follows by summing these two terms together. Q.E.D.

When $n = 2$, the above formula can be further simplified. In fact,

$$T_{1\rightarrow 2} = a_{21} \sigma'_{22} \cdot \sigma_{12} + a_{22} \sigma'_{22} \cdot \sigma_{22} - a_{22}.$$  

In this case, $\sigma'_{22} = 1/\sigma_{22}$, so

$$T_{1\rightarrow 2} = a_{21} \frac{\sigma_{12}}{\sigma_{22}},$$  

just as expected (cf. [15]).

From above it is easy to see that,

$$T_{1\rightarrow 2..n} \neq \sum_{j=2}^{n} T_{1\rightarrow j}. \quad (18)$$

That is to say, the macrostate of a network is not just a simple addition of the individual states. The equality can hold only when the $n$ components are uncorrelated, i.e., when $\Sigma$ is a diagonal matrix, and hence $\sigma'_{ii} = 1/\sigma_{ii}$ and $\sigma'_{ij} = 0$ for $i \neq j$. Indeed, in this case, the $n$ components are just independent units; they do not form a network.
B. The impact of $x_1$ on $x_1$

We know information flow or causality is asymmetric between two entities; that is to say, the contribution of $x_1$ to the rest of the network is generally different from that the other way around. For late reference, we here briefly present the result of the information flow from $x_1$ to $x_1$, though it is not needed in this study.

From \[15\],
\[
\frac{dH_1}{dt} = -E \left[ F_1 \frac{\partial \log \rho_1}{\partial x_1} \right] - \frac{1}{2} E \left[ g_{11} \frac{\partial^2 \log \rho_1}{\partial x_1^2} \right]. \tag{19}
\]

Now if we modify the system on the infinitesimal interval $[t + \Delta t]$ by freezing $(x_2, x_3, ..., x_n)$, and follow the above derivation, we finally arrive at the time rate of change of the marginal entropy of $x_1$ with the effect of $(x_2, x_3, ..., x_n)$ excluded is
\[
\frac{dH_{1,2..n}}{dt} = E \left( \frac{\partial F_1}{\partial x_1} \right) - \frac{1}{2} E \left( g_{11} \frac{\partial^2 \log \rho_1}{\partial x_1^2} \right) - \frac{1}{2} E \left( \frac{1}{\rho_1} \frac{\partial^2 g_{11} \rho_1}{\partial x_1^2} \right). \tag{20}
\]

So the information flow from $x_1$ to $x_1$ is
\[
T_{2..n \rightarrow 1} = \frac{dH_1}{dt} - \frac{dH_{1,2..n}}{dt} = -E \left[ F_1 \frac{\partial \log \rho_1}{\partial x_1} + \frac{\partial F_1}{\partial x_1} \right] + \frac{1}{2} E \left[ \frac{1}{\rho_1} \frac{\partial^2 g_{11} \rho_1}{\partial x_1^2} \right] \tag{21}
\]

A seemingly surprising observation is that this is precisely the same in form as that for 2D systems (see \[15\]), although here the dimensionality can be larger than 2. This does make sense, as we are splitting the system into two subsystems, one with $x_1$, another with a collection of $n - 1$ units. In the meantime, this generally differs in form from those individual information flow formulas for systems with $n > 2$ (see \[9\]).

III. MAXIMUM LIKELIHOOD ESTIMATION

Given a system like (1), we can rigorously evaluate the information flows among the components. Now suppose, instead of the system, what we have are just $n$ time series with $K$ steps, $K \gg n$, \{x_1(k)\}, \{x_2(k)\}, ..., \{x_n(k)\}. We can estimate the system from the series, and then apply the information flow formula to fulfill the task. Assume a linear model as shown above, and assume $m = 1$. following
Liang (2014) [8], the maximum likelihood estimator of $a_{ij}$ is equal to
the least-square solution of the following over-determined problem

$$
\begin{pmatrix}
1 & x_1(1) & x_2(1) & \ldots & x_n(1) \\
1 & x_1(2) & x_2(2) & \ldots & x_n(2) \\
1 & x_1(3) & x_2(3) & \ldots & x_n(3) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
1 & x_1(K) & x_2(K) & \ldots & x_n(K)
\end{pmatrix}
\begin{pmatrix}
f_i \\
a_{i1} \\
a_{i2} \\
\vdots \\
a_{in}
\end{pmatrix}
=
\begin{pmatrix}
\dot{x}_i(1) \\
\dot{x}_i(2) \\
\dot{x}_i(3) \\
\vdots \\
\dot{x}_i(K)
\end{pmatrix}
$$

where $\dot{x}_i(k) = (x_i(k + 1) - x_i(k))/\Delta t$ ($\Delta t$ is the time stepsize), for
$i = 1, 2, \ldots, n, k = 1, \ldots, K$. Use overbar to denote the time mean over
the $K$ steps. The above equation is

$$
\begin{pmatrix}
1 & \bar{x}_1 & \bar{x}_2 & \ldots & \bar{x}_n \\
0 & x_1(2) - \bar{x}_1 & x_2(2) - \bar{x}_2 & \ldots & x_n(2) - \bar{x}_n \\
0 & x_1(3) - \bar{x}_1 & x_2(3) - \bar{x}_2 & \ldots & x_n(3) - \bar{x}_n \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & x_1(K) - \bar{x}_1 & x_2(K) - \bar{x}_2 & \ldots & x_n(K) - \bar{x}_n
\end{pmatrix}
\begin{pmatrix}
f_i \\
a_{i1} \\
a_{i2} \\
\vdots \\
a_{in}
\end{pmatrix}
=
\begin{pmatrix}
\bar{x}_i \\
\dot{x}_i(2) - \bar{x}_i \\
\dot{x}_i(3) - \bar{x}_i \\
\vdots \\
\dot{x}_i(K) - \bar{x}_i
\end{pmatrix}
$$

Denote by $\mathbf{R}$ the matrix

$$
\begin{pmatrix}
x_1(2) - \bar{x}_1 & x_2(2) - \bar{x}_2 & \ldots & x_n(2) - \bar{x}_n \\
\vdots & \vdots & \ddots & \vdots \\
x_1(K) - \bar{x}_1 & x_2(K) - \bar{x}_2 & \ldots & x_n(K) - \bar{x}_n
\end{pmatrix}
$$

$s$ the vector $(x_i(2) - \bar{x}_i, \ldots, x_i(K) - \bar{x}_i)^T$, and $\mathbf{a}_i$ the row vector
$(a_{i1}, \ldots, a_{in})^T$. Then $\mathbf{R}\mathbf{a}_i = s$. The least square solution of $\mathbf{a}_i$, $\hat{\mathbf{a}}_i$, solves

$$
\mathbf{R}^T\mathbf{R}\hat{\mathbf{a}}_i = \mathbf{R}^T s.
$$

Note $\mathbf{R}^T\mathbf{R}$ is $K\mathbf{C}$, where $\mathbf{C}$ is the covariance matrix. So

$$
\begin{pmatrix}
\hat{a}_{i1} \\
\hat{a}_{i2} \\
\vdots \\
\hat{a}_{in}
\end{pmatrix}
= \mathbf{C}^{-1}
\begin{pmatrix}
c_{1,di} \\
c_{2,di} \\
\vdots \\
c_{n,di}
\end{pmatrix}
$$

(22)

where $c_{j,di}$ is the covariance between the series $\{x_j(k)\}$ and $\{(x_i(k + 1) - x_i(k))/\Delta t\}$.

So finally, the mle of $T_{1\rightarrow 2,n}$ is

$$
\hat{T}_{1\rightarrow 2,n} = \sum_{i=2}^{n} \left[ \sum_{j=2}^{n} c_{ij}' \left( \sum_{k=1}^{n} \hat{a}_{ik}c_{kj} \right) - \hat{a}_{ii} \right],
$$

(23)

13
where $c'_{ij}$ is the $(i, j)^{th}$ entry of $\tilde{C}^{-1}$, and

$$
\tilde{C} = \begin{pmatrix}
1 & 0 & 0 & \ldots & 0 \\
0 & c_{22} & c_{23} & \ldots & c_{2n} \\
0 & c_{23} & c_{33} & \ldots & c_{3n} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
0 & c_{2n} & c_{3n} & \ldots & c_{nn}
\end{pmatrix}.
$$

(24)

Denoting by $\hat{A}$ the matrix with entries $(\hat{a}_{ij})$, Eq. (23) can be more succinctly written as:

$$
\hat{T}_{1\rightarrow2..n} = \text{Tr}\left[\tilde{C}^{-1}(\hat{A}\hat{C})^T\right] - \text{Tr}\left[\hat{A}\right].
$$

(25)

Here $\text{Tr}\left[Q\right]$ means the trace of a matrix with the first term removed. That is to say, it is defined such that, for matrix $Q$,

$$
\text{Tr}\left[Q\right] = \text{Tr}\left[Q\right] - Q(1, 1).
$$

Note this is made possible by the form of $\tilde{C}$ (with its special form in $1^{st}$ row and $1^{st}$ column); otherwise the trace of the product of two matrices, say, $P_{n\times n}Q_{n\times n} \equiv R_{n\times n}$, is generally not equal to $\text{Tr}[P(2 : n, 2 : n)Q(2 : n, 2 : n)] + R(1, 1)$.

IV. APPLICATION TO A NETWORK OF COUPLED STUART-LANDAU OSCILLATORS

In this section we put (23) to application to a network with $N$ nodes, each made of a Stuart-Landau oscillator[17]. This has been used to model many biological networks for phenomena such as circadian rhythms, synchronized neuronal firing, and spatiotemporal activity in the heart and the brain (see [7] for more examples). For the purpose of demonstration, here a small number $N = 6$ is chosen. Let the complex state variable of the $j^{th}$ oscillator be $z_j$. It is defined as (see, e.g., [18][7])

$$
\frac{dz_j}{dt} = (\alpha_j + i\Omega_j - |z_j|^2) z_j + \frac{K}{N} \sum_{k=1}^{N} \Lambda_{jk}(z_k - z_j) + \nu \dot{w}_j, \quad j = 1, ..., N
$$

(26)

where $i = \sqrt{-1}$, $\Omega_j$ are the frequencies, $\alpha_j$ are control parameters, and $(\Lambda)$ is the adjacency matrix. Here the coupling coefficient $K$ is chosen to be 1. The notation generally follows that in [7]; the difference lies in
an \(\Omega\) varying oscillator by oscillator, and an additional stochastic term 
\(\nu \dot{w}_j\), where \(w_j\) is a standard Wiener process, and \(\nu\) the stochastic perturbation amplitude. We add some weak stochasticity for convenience (see below). If \(K = 0\) and \(\nu = 0\), the oscillators are Stuart-Landau oscillators; a positive \(\alpha_j\) yields an oscillating state, whereas a negative \(\alpha_j\) disable the oscillator. In this study, \(K = 1\), \(\Omega_j = j/2\), \(j = 1, \ldots, N\), are fixed throughout. \(\alpha_j\) may be 1 or \(-3\), depending on whether \(z_j\) is activated or switched off. The adjacency matrix is chosen such that 
\(\Lambda_{2k} = \Lambda_{k2} = 0, k = 1, 3, 4; \Lambda_{1k} = \Lambda_{k1} = 0, k = 4, 6\), and for all other \((j, k)\), \(\Lambda_{jk} = 1\). The resulting network is sketched in Fig. 1. Obviously, \(z_5\) is a highly connected node, or hub; second to it is \(z_6\). \(z_1\) and \(z_2\) are two sparsely connected nodes.

FIG. 1: A schematic of the network of coupled oscillators. For the sake of clarity, in this study only the 6-node (red) subnetwork is considered.

Equation (26) is discretized and solved using the second order Runge-Kutta scheme. The system is initialized with random values, integrated forward with a time stepsize of \(\Delta t = 0.1\). Without coupling, the individual oscillators operate on their own, each exhibiting a periodic series with a distinct frequency. Shown in Fig. 2a are the active (solid) and inactive (dashed) modes for \(z_1\) when \(\nu = 0\). Fig. 2b displays the corresponding cases when \(\nu = 0.1\). We need this slightly perturbed system because, as seen in Fig. 2a, the trajectories are too regular (periodic), only leaving on the Poincar’e plane one point. In other words, they contain no information, making the information flow problem singular. Recently it is found this is actually an extreme case[20],
and hence can be handled by perturbing the system slightly with weak stochasticity. (In real systems, noises are ubiquitous.) The Fig. 2b approximate well its deterministic case, Fig. 2a, except for some weak ripples superimposed on the curves. So it is reasonable to believe that the addition of the weak perturbation can be used to compute the information flow for the original system.

![Fig. 2](image)

**FIG. 2:** Time series of a single oscillator \( z_1 \) without coupling \((K = 0)\). (a) No noise; (b) weak stochasticity applied \((\nu = 0.1)\). Only the real parts are drawn.

Figure 3 shows the time series of the six coupled oscillators. In (a), all of them are on. As seen, though the frequencies \( \Omega_j \) differ, the six oscillators work together to produce completely synchronized oscillations (see [19] for optimum synchronizations). To assess the importance of a node, a usual practice is to delete it from the network and observe the response. In Figs. 3b-g, shown are the respective responses when \( z_1-z_6 \) are turned off respectively. Obviously, with only one node failure the network is still alive. But one can see that the impact of \( z_5 \) is significantly larger than others, while that from \( z_1 \) is by far the least. In Fig. 3h, when \( z_5 \) and \( z_2 \) are disabled, then the entire network gradually dies, though in this case \( \alpha_1, \alpha_3, \alpha_4, \alpha_6 \) are still positive.

As mentioned in the introduction, the above assessment by preferential removal of designated node(s) may not be feasible for many networks in nature, neuronal networks in particular. Now use formula (23) to estimate the information flow from the individual oscillators to the network. To begin, note that each \( z_j \) actually has two components; so they should be taken as two time series. That is to say, the dynamical system has a dimensionality of \( 2 \times N \). The remaining computation is straightforward. We generate series with 5000 steps, with the first 100 steps discarded (to ensure stationarity). The computed results are (units in nats per unit time; values may differ slightly due to the random initialization):
FIG. 3: Time series of the six coupled oscillators $z_j$ (only the real parts of $z_j$ are drawn). (a) All oscillators are active; (b) $z_1$ inactive (all others are active; same below); (c) $z_2$ inactive; (d) $z_3$ inactive; (e) $z_4$ inactive; (f) $z_5$ inactive; (g) $z_6$ inactive; (h) both $z_2$ and $z_5$ are inactive.

| $\hat{T}_1 \to \text{network} \hat{T}_2 \to \text{network} \hat{T}_3 \to \text{network} \hat{T}_4 \to \text{network} \hat{T}_5 \to \text{network} \hat{T}_6 \to \text{network}$ | 0.66 | 1.30 | 2.11 | 2.50 | 3.07 | 3.03 |

By comparison $z_5$ and $z_6$ are most important; second to them are $z_3$ and $z_4$. $z_1$ and $z_2$ are least important. The result is just as that as illustrated in Fig. 3. From out common intuition, this makes sense, too. As we can check from Fig. 1, $z_5$ and $z_6$ are the hubs, whereas $z_1$ and $z_2$ are sparsely connected.

However, if there exist directed links and/or localized weights (e.g., [19]) in the network, hubs need not always be the most crucial units. To see this, let $\Lambda_{52} = 10$, $\Lambda_{62} = 5$. The computed result is tabulated as follows:
So now the most important node is $z_2$, though it is sparsely connected! And, the impact from $z_6$ has been greatly reduced.

To see whether this is indeed the case, we do the node removal experiments again. Indeed, if $z_2$ is deteriorated or suppressed, the whole network becomes silent, as shown in Fig. 4c. The result is hence validated.

| $T_1\rightarrow\text{network}$ | $T_2\rightarrow\text{network}$ | $T_3\rightarrow\text{network}$ | $T_4\rightarrow\text{network}$ | $T_5\rightarrow\text{network}$ | $T_6\rightarrow\text{network}$ |
|-------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|-------------------------------|
| 0.50                          | 4.00                          | 1.92                          | 2.10                          | 2.55                          | 0.77                          |

FIG. 4: As Fig. 3, but with weighted and directed links.

V. SUMMARY

A quantitative evaluation of the contribution of individual units in producing the collective behavior of a complex network is important in that is allows us to gain an understanding of which units determine the
vulnerability of the network. In this study, we show that a natural measure is the information flow from the unit in concern to the entire network. A formula is derived, and its maximum likelihood estimator provided. The results are summarized henceforth for easy reference.

For a network modeled with an $n$-dimensional continuous-time dynamical system

$$\frac{dx}{dt} = F(x, t) + B(x, t)\dot{w},$$

the information flow from node $x_1$ to the network $x_2, x_3, \ldots, x_n$ is

$$T_{1\to 2..n} = -E \left[ \sum_{i=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial F_i}{\partial x_i} \right] + \frac{1}{2} E \left[ \sum_{i=2}^{n} \sum_{j=2}^{n} \frac{1}{\rho_{2..n}} \frac{\partial^2 g_{ij}}{\partial x_i \partial x_j} \right].$$

When only time series are available, under the assumption of linearity, the maximum likelihood estimator of $T_{1\to 2..n}$ is

$$\hat{T}_{1\to 2..n} = Tr_\eta \left[ \tilde{C}^{-1}(\hat{A}C)^T \right] - Tr_\eta \left[ \tilde{A} \right].$$

In the equation, $Tr_\eta$ means the trace of a matrix with the first term removed, $C = (c_{ij})$ is the covariance matrix, $\tilde{C}$ is equal to $C$ except $\tilde{c}_{1,1} = 1, \tilde{c}_{j,1} = \tilde{c}_{1,j} = 0, j = 2, 3, \ldots, n$. $\tilde{A} = (\hat{a}_{ij})$ has entries

$$\begin{pmatrix} \hat{a}_{i1} \\ \hat{a}_{i2} \\ \vdots \\ \hat{a}_{in} \end{pmatrix} = C^{-1} \begin{pmatrix} c_{1,di} \\ c_{2,di} \\ \vdots \\ c_{n,di} \end{pmatrix}, \quad i = 1, 2, \ldots, n,$$

where $c_{j,di}$ is the covariance between the series $\{x_j(k)\}$ and $\{(x_i(k + 1) - x_i(k))/\Delta t\}$. Observe that this “cumulative information flow” is not equal to the sum of the information flows to other individual units, reflecting the collective phenomenon that a group is not the addition of the individual members.

The above formula has been put to application to a network consisting of Stuart-Landau oscillators. It is shown that the node with largest information flow is indeed most crucial for the network. Its deterioration or suppression will cause the whole network to cease to function. An observation is: depending on the topology, such a node may not be a hub; on the contrary, it could be some sparsely connected, low-degree node. This study is expected to be useful in identifying clues to the mystery why initially small shocks at some nodes may trigger a massive, global shutdown of the entire network.
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