Invariant Multiparameter Sensitivity to Characterize Dynamical Systems on Complex Networks

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The behavior of systems is determined by the parameters. Because we seldom know the detailed structure of a system, metrics of parameter sensitivity should be independent of how we model the system. We formulate a new parameter sensitivity metric, which we refer to as "invariant multiparameter sensitivity" (IMPS) because it gives the same result for a class of equivalent models of a system. To investigate the property of IMPS, we firstly apply IMPS to resistor circuits and linear dynamical systems. To examine the dependence of IMPS on network structures, we secondly apply IMPS to nonlinear systems on complex networks. We find that the IMPS of networks of phase oscillators is essentially independent of the number of oscillators. We examine the network-structure dependence of IMPS using a simplified solvable model.

1. Introduction

Over the past few decades, research has increasingly focused on social, biological, economical, ecological, and geological systems.[1–5] The outputs of these systems depend on parameters. In these systems, the parameters may fluctuate stochastically and undergo long-term drift. Thus, understanding the effect of variations in the parameters on the system outputs is vital for understanding their dynamics.[6,7] For example, this approach is used to characterize electric circuits that are insensitive to variations in individual circuit elements.[7–9]

In this study, we focus on the changes in the response of system outputs when the parameters are changed; this relation is referred to as the "parameter sensitivity" of the system. Parameter sensitivity has been intensively studied in circuit theory, particularly in resistor–capacitor networks.[7–10] Although parameter sensitivity was originally proposed to evaluate the sensitivity of electric circuits, it has also been used in many other fields, such as biology,[11–13] ecology,[14] and economics.[15] Previous studies have proposed several metrics for

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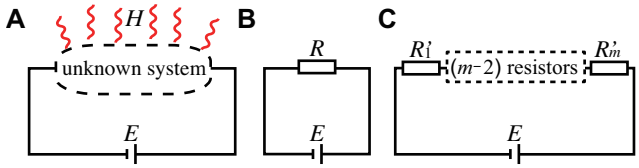

Fig. 1. (Color online) Unknown heating system (A) and series resistor models (B,C). The models B and C are electrically equivalent when $R'_1 + R'_2 + \cdots + R'_m = R$.

parameter sensitivity.[16,17] Single parameter sensitivity (SPS) is the ratio of the change in output to the change in parameter.[18] Since most systems have more than one parameter, generalizing SPS to multiple parameters is the next logical step. Multiparameter sensitivity (MPS) is a generalization of SPS for multiple parameters.[18] MPS is defined as the square root of the sum of the squares of SPSs of the system. MPS has been used in analyzing networks with circuit elements.[9,18,19] In biology, MPS was used in clarifying how the integration of molecular components generates robust systems such as the *Escherichia coli* heat-shock response system and the *Drosophila melanogaster* circadian clock.[11]

The parameter sensitivity of a system is often numerically estimated by quantifying the parameter sensitivity of its models.[8,11–13] Because, in most cases, we do not know the structures and dynamics of systems completely, a wide variety of models are proposed for a single system. As an example, let us assume that we want to quantify the parameter sensitivity of the system of Fig. 1A. When connected to a voltage source E, this system exhibits heat flow H. Here, we assume that this system comprises linear resistors. Even under this assumption, this system can be modeled by a large number of electric circuit models, such as those in Figs. 1B and 1 C. Unfortunately, as will be shown in the next section, MPS gives different results for the models in Figs. 1B and 1 C, which are electrically equivalent models of a single system of Fig. 1A. Since MPS depends on the choice of the models, we cannot quantify the parameter sensitivity of the system using MPS.

To address this problem, we propose a new sensitivity metric, which we call "invariant multiparameter sensitivity" (IMPS). In Sect. 2, we briefly review previously proposed sensitivity metrics and then define IMPS. We use the example of serial resistor models to present "invariance," which is an important property of IMPS. In Sect. 3, IMPS for linear dynamical systems is examined. Furthermore, we study the IMPS for phase oscillator models on complex networks in Sect. 4. IMPS is suggested to vary according to network structures. Finally, in Sect. 5, we summarize the main results and discuss the potential applications and limitations of IMPS. Detailed derivations can be found in Supplemental Materials.[20]

2. Invariant Multiparameter Sensitivity

Models of dynamical systems are expressed by the first-order differential equations

$$\dot{\vec{x}} = F\left(t, \vec{x}, \vec{p}\right), \tag{1}$$

where t is the time, $\vec{x} = [x_1, x_2, x_3, \ldots, x_n]$ is the state variable vector, and $\vec{p} = [p_1, p_2, p_3, \ldots, p_m]$ is the parameter vector. Let q be the output whose sensitivity to parameters we want to quantify. Here, the output can be any value derived from the system, such as oscillation period, cell growth rate, or energy consumption. For a given output q, the single parameter sensitivity with respect to the parameter p_i, which we call SPS_i, is defined as

$$\mathrm{SPS}_i = \frac{p_i}{q}\frac{\partial q}{\partial p_i} = \frac{\partial \ln q}{\partial \ln p_i}. \tag{2}$$

SPS_i is the ratio of the change in the output q to the change in the parameter p_i.[18] SPS_i does not quantify the sensitivity of q with respect to any other parameters. Generalizing SPS to multiple parameters, Goldstein and Kuo defined MPS as the L2 norm of SPSs:[18]

$$\mathrm{MPS}^2 = \sum_{i=1}^{m} \mathrm{SPS}_i^2. \tag{3}$$

MPS has been used to quantify the sensitivity of the output to changes in the entire parameter set of models.[9,18,19] However, MPS often gives different results for two equivalent models of a system. Consider a model of a circuit with one resistor R, as shown in Fig. 1B. Let H denote the heat flow from the circuit and let E denote the voltage of the voltage source. We assume that the heat flow $H = E^2/R$ is the output of this model. Because the SPS of this circuit with respect to R is unity, the MPS is also unity. A current-voltage relationship identical to that of Fig. 1B can also be implemented by equivalent circuits, such as that shown in Fig. 1C (assuming $R'_1 + R'_2 + \ldots + R'_m = R$). The MPS of the circuit of Fig. 1C is given by

$$\begin{aligned} \mathrm{MPS}^2 &= \sum_{i=1}^{m} \left(\frac{R'_i}{H}\frac{\partial H}{\partial R'_i}\right)^2 \\ &= \sum_{i=1}^{m} \frac{R'^2_i}{R^2}. \end{aligned} \tag{4}$$

Hence, the MPS of this model decreases as m increases.

In contrast, the L1 norm of SPSs of the circuit for Fig. 1C is given by

$$\begin{aligned} \sum_{i=1}^{m} |\mathrm{SPS}_i| &= \sum_{i=1}^{m} \left|\frac{R'_i}{H}\frac{\partial H}{\partial R'_i}\right| \\ &= 1, \end{aligned} \tag{5}$$

which equals the L1 norm of SPSs for the circuit of Fig. 1B. Thus, we introduce a new metric

IMPS, which is the sum of all absolute values of SPSs:

$$\mathrm{IMPS} = \sum_{i=1}^{m} |\mathrm{SPS}_i| \,. \tag{6}$$

The IMPS of the circuit is constant, regardless of m because the output H is a homogeneous function of degree -1 of resistances $R_1, R_2, \ldots$, and R_m. Indeed, assuming that the output $q(p_1, p_2, p_3, \ldots, p_m)$ is a homogeneous function of the degree k and that the SPSs in Eq. (6) have the same sign, we obtain

$$\begin{aligned} \mathrm{IMPS} &= \sum_{i=1}^{m} \left| \frac{p_i}{q} \frac{\partial q}{\partial p_i} \right| \\ &= |k| \,, \end{aligned} \tag{7}$$

where we use Euler's theorem

$$\sum_{i=1}^{m} p_i \left(\frac{\partial q}{\partial p_i} \right) = kq(p_1, p_2, p_3, \ldots, p_m). \tag{8}$$

This is also the case with equivalent circuits of resistors in parallel. These results suggest that IMPS is independent of the models, and may be a metric for quantifying the sensitivity of the system itself rather than the model. The IMPSs are the same for all models satisfying the following conditions: (i) the output is a homogeneous function of the parameters and (ii) the SPSs have the same sign. These conditions are not necessarily satisfied. However, in the following, we show that these conditions are approximately satisfied in several models of linear and nonlinear dynamics.

3. Linear Dynamics

There are many systems that can be modeled by elements interacting with each other.[21–24] As a simple example of these models, we examine a model consisting of N particles. Assume that particle i has the position x_i and the velocity $\dot{x}_i$, and is attracted to other particles via the connection weight matrix $\mathbf{W} = (W_{ij})$. The matrix $\mathbf{W}$ is symmetric, has no negative elements, and is assumed to define a connected graph of particles. Then, the dynamics are defined by

$$\dot{x}_i = \frac{dx_i}{dt} = b_i + \sum_{j=1}^{N} W_{ij}(x_j - x_i), \tag{9}$$

where b_i is the velocity of the particle i with no interaction. The velocity b_i is drawn from a unit normal distribution. The positions of the particles converge to fixed points. The variance V of the positions at the steady state is used as the output of the model, whose sensitivity is to be measured. We assume a connected graph because the variance cannot be defined when particles become disconnected.

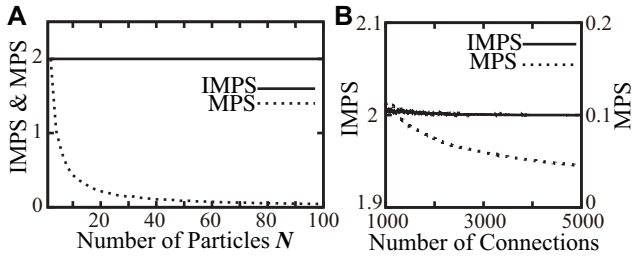

Fig. 2. IMPS (solid line) and MPS (dashed line) for linear dynamical models. Panel A shows IMPS and MPS as functions of N. Panel B shows IMPS and MPS as functions of the number of connections for $N = 100$.

By using the Laplacian matrix $\mathbf{L}$ of a weighted graph[25] defined by the connection weight matrix $\mathbf{W}$, we obtain

$$\begin{aligned} \mathrm{IMPS} &= \frac{1}{N}\sum_{\langle ij\rangle}\left|-\frac{W_{ij}}{V}\vec{b}^{T}\tilde{\mathbf{L}}^{-1}\left(\frac{\partial\tilde{\mathbf{L}}}{\partial W_{ij}}\tilde{\mathbf{L}}^{-1}+\tilde{\mathbf{L}}^{-1}\frac{\partial\tilde{\mathbf{L}}}{\partial W_{ij}}\right)\tilde{\mathbf{L}}^{-1}\vec{b}\right| \\ &\quad +\frac{1}{N}\left|-\frac{\beta}{V}\vec{b}^{T}\tilde{\mathbf{L}}^{-1}(\mathbf{1}\tilde{\mathbf{L}}^{-1}+\tilde{\mathbf{L}}^{-1}\mathbf{1})\tilde{\mathbf{L}}^{-1}\vec{b}\right|, \end{aligned} \tag{10}$$

where $\langle\rangle$ indicates the summation over the connected particle pairs, and $\tilde{L}_{ij} = L_{ij} + \beta$. $\beta \neq 0$ is introduced so that $\tilde{\mathbf{L}}$ is invertible. IMPS is independent of β. The detailed derivation is given in Supplemental Materials Analysis S1.[20] By assuming that all SPSs have the same sign, we obtain IMPS $= 2$ because the variance is a homogeneous function of degree -2, regardless of network size and the structure given by the connection weight matrix $\mathbf{W}$ as shown in Eq. (S-20).

Let us examine whether the result IMPS $= 2$ holds in numerical simulations. Figure 2A shows that this relation holds for the network of all-to-all coupling, $W_{ij} = 0$ for $i = j$ and $W_{ij} = 1$ otherwise, for a wide range of N. This suggests that all SPSs have the same sign in this model. In contrast, the MPS decreases as N increases (Fig. 2A).

In the simulation of Fig. 2B, we start from a fully connected system of size $N = 100$ and eliminate a connection at each step. We confirmed that $\mathbf{W}$ constituted a connected graph. Thus, the graph at each step is an Erdős–Rényi random graph.[26] The IMPS and MPS are shown in Fig. 2B as functions of the number of connections. This figure shows that MPS depends much more strongly on the number of connections than IMPS. Therefore, these results indicate that the condition that all SPSs have the same sign is almost satisfied. Moreover, these results indicate that, for these linear models, the IMPS quantifies how sensitively the system's output, that is, the variance of the particle positions, changes in response to a parameter change in a manner that is independent of N and the number of connections.

4. Phase Oscillator Networks

Let us consider a system of oscillatory elements on a network. Oscillatory elements are often modeled by phase oscillators.[21,27,28] Because the precise structure of a network may be unknown to us, to investigate how IMPS is affected by the choice of network structure used to model the system, we compare IMPSs of phase oscillators on the three types of network, that is, Barabási–Albert, regular random, and Watts–Strogatz networks. Now, consider a model of N oscillators connected to each other by the adjacency matrix $\mathbf{A} = (A_{ij})$, where $A_{ij} = 1$ for connected pairs and $A_{ij} = 0$ otherwise. The dynamics of the oscillator i are described by

$$\frac{d\theta_i}{dt} = \omega_i + \sum_{j=1}^{N} K_{ij} \sin(\theta_j - \theta_i), \tag{11}$$

where ω_i is the natural frequency of the oscillator i and K_{ij} is the element (i, j) of the connection weight matrix $\mathbf{K}$.[21,29] For the numerical simulation, we use $\mathbf{K} = \alpha\mathbf{A}$, where $\alpha > 0$ is the coupling strength, and draw the natural frequency ω_i from a unit normal distribution. Without loss of generality, we can assume that $\sum_{i=1}^{N} \omega_i = 0$. For α, we use a sufficiently large value so that all phase oscillators are phase locked. We use the circular variance V_c of the oscillators in the phase-locked state[30] as the output:

$$V_c = 1 - r = 1 - \frac{1}{N}\sqrt{C^2 + S^2}, \tag{12}$$

where r is the Kuramoto order parameter, $C = \sum_{i=1}^{N} \cos\theta_i$, and $S = \sum_{i=1}^{N} \sin\theta_i$.

To simulate phase oscillators on complex networks, we use the adjacency matrices given by Barabási–Albert[31] (a well-known model of scale-free networks) and regular random networks with an average degree of 4. We use output V_c at $t = 100$ for Barabási–Albert and regular random networks. To generate a Barabási–Albert network, we use Gephi complex generators. We start from 2 connected vertices and add a vertex with 2 edges in each step until we have N vertices. We generate regular random networks with degree 4 using the Matlab Random Regular generator. The phases of all oscillators are distributed uniformly at $t = 0$.

By using the implicit function theorem, we derive $\partial V_c/\partial K_{ij}$ [Eq. (S-32)].[20] We calculate the IMPS numerically using Eq. (S-33).[20] Unlike for equivalent electric circuits and linear dynamical models, IMPSs for phase oscillator networks are not constant (Fig. 3). This result is attributed to V_c not being a homogeneous function. Figure 3A shows the results of 10 000 phase oscillators on 5 Barabási–Albert networks and Fig. 3B shows the results of 10 000 phase oscillators on 5 regular random networks generated by different random seeds. The IMPSs converge to 2, as shown in Figs. 3A and 3B. This is because, as the coupling strength α increases, the models can be described by linearized dynamics. The nonlinear dynamics of

Table I. Average path length of oscillator networks ($N = 10\,000$)

	Barabási–Albert	Regular Random	300-connection Rewired Watts–Strogatz	3000-connection Rewired Watts–Strogatz
Mean	5.03	7.73	36.1	10.9
Standard Deviation	2.20×10^{-2}	1.53×10^{-3}	0.343	2.88×10^{-2}

Eq. (11) become the linear dynamics of Eq. (9), and the circular variance of Eq. (12) becomes proportional to the variance in the large α limit.

In Fig. 4, for models on Barabási–Albert networks, we compare the IMPS and MPS as functions of coupling strength α for models with different N values. As shown in Fig. 4A, the IMPSs for models with different N values are close together. In contrast, as shown in Fig. 4B, the MPSs for models with different N values are well separated. IMPSs for models with different N values converge to the same value, 2, for the nonlinear models as well as the linear models.

Next, to examine another type of complex network, we use the adjacency matrices given by Watts–Strogatz networks[1)] with an average degree of 4. We use the output V_c at $t = 200$ for Watts–Strogatz networks. To generate a Watts–Strogatz network,[1)] we start from a regular ring lattice with N vertices; each vertex is connected to 4 neighbors, 2 on each side. We randomly select an edge and rewire one of its endpoints step by step either 300 or 3000 times. The phases of all oscillators at $t = 0$ are drawn from a Gaussian distribution with a mean of 0 and a standard deviation of 0.1.

Figure 3C1 (3C2) shows the IMPS for 10 000 phase oscillators on Watts–Strogatz networks with 300 (3000) of 20 000 connections rewired. Figures 3C1 and 3C2 are generated using different random seeds. For the models on Watts–Strogatz networks, although the IMPS approaches 2 as α increases, the IMPS deviates from 2 more than the IMPS for the models on Barabási–Albert and regular random networks. As shown in Fig. 3C1, the IMPS curves are distributed more widely than those of Figs. 3A and 3B. The result suggests that the IMPS of the models on Watts–Strogatz networks varies from network to network. On the other hand, IMPSs are within a narrower range for Barabási–Albert and regular random networks. For the models on Barabási–Albert and regular random networks, the IMPS converges to 2 from above, whereas, for models on Watts–Strogatz networks, the IMPS converges to 2 from below. These observations suggest that the circular variance for Barabási–Albert and regular random networks changes much more sensitively depending on the coupling strength of each

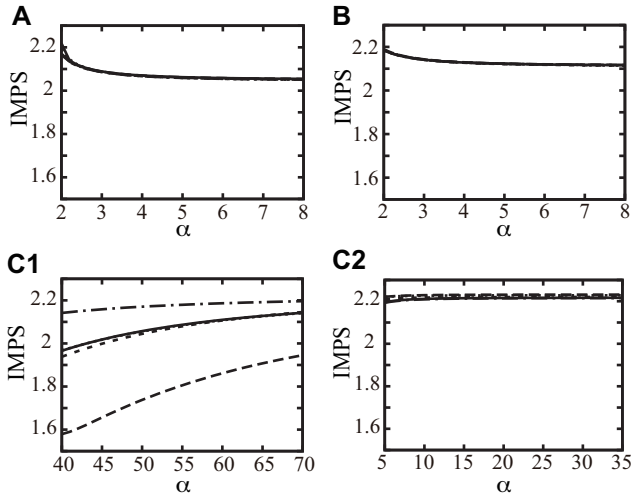

Fig. 3. IMPS for 10 000 oscillators on complex networks. IMPSs for the models on Barabási–Albert (A), regular random (B), and 300-connection rewired Watts–Strogatz (C1), and 3000-connection rewired Watts–Strogatz (C2) networks are shown. In panels A and B, the coupling strength α varies from 2 to 8 in steps of 0.2. In panel C1, α varies from 40 to 70 in steps of 1. In panel C2, α varies from 5 to 35 in steps of 1.

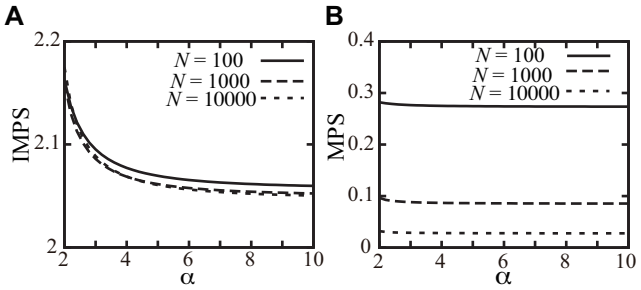

Fig. 4. IMPS and MPS for 100, 1000, and 10 000 oscillators on Barabási–Albert networks. (A) IMPS and (B) MPS as functions of coupling strength α for the models on Barabási–Albert networks. In both panels, the coupling strength α varies from 2 to 10 in steps of 0.2.

vertex than the circular variance for Watts–Strogatz networks when the coupling strength α is small. This implies that IMPS reflects some difference in network structures and network metrics among Barabási–Albert and regular random networks and Watts–Strogatz networks.

To clarify the factor reflected in IMPS, next we examine a solvable oscillator model. Compared with Barabási–Albert and regular random networks, Watts–Strogatz networks have longer average path lengths (Table I). Watts–Strogatz networks have a larger number of long one-dimensional (1-D) lattice like structures (Fig. 5A) than Barabási–Albert and regular random networks. To investigate the effects of 1-D lattice like structures, we simplify a regular 1-D lattice to a path graph, for which all vertices and edges lie on a single straight line

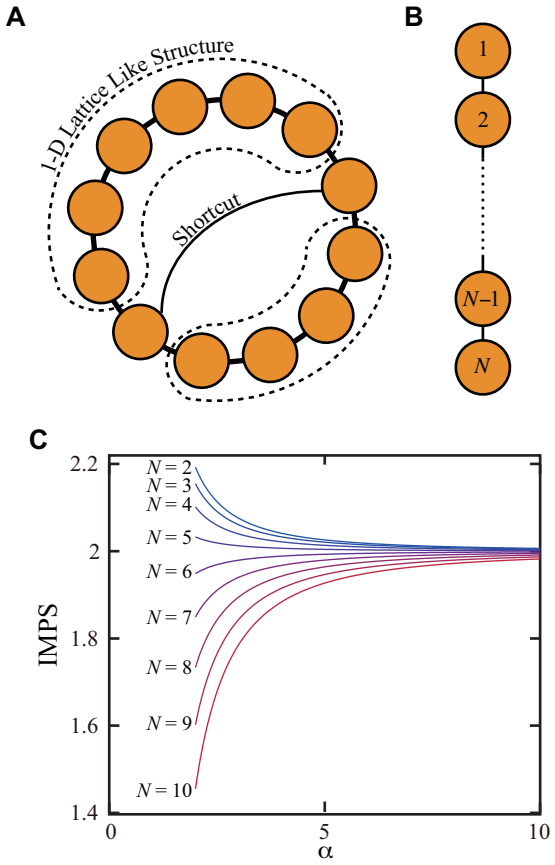

Fig. 5. (Color online) One-dimensional lattice like structure, path graph, and IMPS for path graphs of different lengths. Panel A shows a schematic of a 1-D lattice like structure. Panel B shows a path graph with N vertices. Panel C shows the IMPS for models with different-length path graphs as a function of the coupling strength α. In panel C, the phases of N oscillators are separated by regular intervals.

(Fig. 5B). When N phase oscillators are connected to each other along a path graph and have natural frequencies $-\omega_1 = \omega_N = 1$ and $\omega_i = 0$ for $1 < i < N$, their phases are separated by regular intervals ($\Delta\theta$). IMPSs for the oscillators on different lengths can be obtained as

$$\mathrm{IMPS} = \frac{\tan(\Delta\theta)}{N^2 r(1-r)} \left| \mathrm{Im}\left[\frac{z^N - 1}{z-1} \overline{\left(\frac{-z^N + N(z-1) + 1}{(z-1)^2} \right)} \right] \right|, \tag{13}$$

where r is the Kuramoto order parameter and $z = e^{\mathrm{i}\Delta\theta}$ (see Supplemental Materials Analysis S3 for derivation[20]). As shown in Fig. 5C, the length of the path graph determines whether the IMPS converges from above or below. The models of shorter (longer) path graphs correspond to models on Barabási–Albert and regular random networks (Watts–Strogatz networks). To further examine how the dependence of IMPS on α is affected by the average path length, we plot the difference between IMPS for a small α and that for a large α (Fig. S1).[20] As is consistent with Fig. 5C, the correlation coefficient r between the average path length and

IMPS($\alpha = 10$) − IMPS($\alpha = 100$) on 50 Watts–Strogatz networks ($N = 1000$, rewiring probability= 0.05) is negative ($r = -0.43$, $p < 0.01$). Other network metrics such as diameter and radius are also correlated to IMPS's difference. On the other hand, for Barabási–Albert networks, the average path length is not significantly correlated to IMPS($\alpha = 2.5$)−IMPS($\alpha = 100$), probably owing to the narrow range of the average path length of randomly generated 50 Barabási–Albert networks ($N = 1000$). These observations suggest that the networks with shorter average path lengths make the model more sensitive to changes in the coupling strength of each vertex.

5. Discussion

In this paper, we reviewed the previously proposed metrics SPS and MPS, which quantify the sensitivity of the output to the values of parameters. We formulated an improved metric called IMPS, which we applied to series-resistor circuits and linear dynamical systems. By calculating the IMPS for series-resistor circuits, we found that IMPS gives identical results for equivalent circuits of Figs. 1B and 1C. The analysis and simulation of linear dynamical models revealed that IMPS is less dependent on the number of particles in the linear dynamical model. We also calculated IMPS for nonlinearly coupled phase oscillators on Barabási–Albert, regular random, and Watts–Strogatz networks. In all of these cases, the IMPS converges to values close to 2. In the limit of a large coupling strength, IMPS is less dependent on the type of network, that is, the Barabási–Albert network, regular random network, Watts–Strogatz network, and path graph. However, for a small coupling strength, IMPSs differ among the types of network used to model the unknown system. Moreover, for a small coupling strength, average path length negatively correlates to IMPS. Thus, for systems of phase oscillators on networks, our results show that the system with a shorter average path length is more sensitive to parameter changes.

The IMPS gives identical results for equivalent circuits (Fig. 1). The invariance of IMPS was previously reported only for resistor–capacitor networks.[7–10] The analysis of the circuits indicates that dividing an element into several elements or combining several elements into a single element does not change the IMPS. This is also the case with the linear and nonlinear dynamical systems. These results suggest that IMPS can be a more appropriate metric than MPS in quantifying the sensitivity of unknown systems, because the precise number of elements in the system in question is often unknown. However, the conditions for the invariance of IMPS may be satisfied only in a limited class of systems.

To use IMPS to compare the sensitivity of various systems, two points must be considered:

(i) IMPS depends on the shift of the zeroes of parameters and (ii) IMPS depends on the dimension of the units of parameters. As an example of the first point, assume the pressure P as the output of a system consisting of an ideal gas in a cuboid. The ideal gas formula is

$$P = \frac{nRT}{V}, \tag{14}$$

where V is the volume of the gas, n is the number of moles of the gas in the cuboid, R is the ideal gas constant, and T $[K]$ is the absolute temperature in Kelvin of the gas. Here, we assume that R is a constant and n, T, and V are the parameters. The IMPS for this model is 3. If we give the temperature C in Celsius, we have $T = C + 273$. The IMPS for this model expressed in Celsius is $2+|\frac{C}{C+273}|$. As an example of the second point, denote the width, depth, and height of the cuboid by w, d, and h, respectively. This gives

$$P = \frac{nRT}{wdh}. \tag{15}$$

The IMPS for this model expressed in terms of n, T, w, d, and h is 5. Thus, the points of zeroes of the parameters and the dimensions of units should be consistent between the models describing systems. SPS and MPS also suffer from the same difficulty.

To summarize, in this paper, we investigated the IMPS with respect to the output of linear and nonlinear models that can be approximately linearized. In strongly nonlinear systems, such as chaotic systems, how their nonlinearity is reflected in IMPS should be examined. In addition, the relationship between IMPS and the Lyapunov exponent is of interest. Future work should also consider the IMPS of other types of nonlinear system.

Acknowledgment

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