Supplemental Materials for Invariant Multiparameter Sensitivity to Characterize Dynamical Systems on Complex Networks

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Analysis S1: Linear Dynamical Model

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Let x_i be the position of particle i and b_i be its velocity with no interaction. The dynamics are described by

$$\dot{x}_i = b_i + \sum_{j=1}^N W_{ij} \left(x_j - x_i \right),$$
(S-1)

where the connection weight matrix **W** is a symmetric matrix, and $W_{ij} \ge 0$. By using a moving coordinate system, we can assume

$$\sum_{i=1}^{N} b_i = 0 \tag{S-2}$$

without loss of generality. In this case, we can assume that the mean of x_i is 0. In a matrix expression, we have

$$\dot{\vec{x}} = \vec{b} + \mathbf{W}\vec{x} - \mathbf{W}^d\vec{x},\tag{S-3}$$

where

$$\mathbf{W}^{d} = \begin{pmatrix} \sum_{j=1}^{N} W_{1j} & 0 & 0 & \cdots & 0 \\ 0 & \sum_{j=1}^{N} W_{2j} & 0 & \cdots & 0 \\ 0 & 0 & \sum_{j=1}^{N} W_{3j} & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & \sum_{j=1}^{N} W_{Nj} \end{pmatrix}.$$
 (S-4)

Because the Laplacian matrix ${\bf L}$ defined by

$$\mathbf{L} = \mathbf{W}^d - \mathbf{W} \tag{S-5}$$

is non-negative definite, the positions of the particles converge to fixed points. After the convergence, we have

$$\dot{\vec{x}} = \vec{b} - \mathbf{L}\vec{x} = 0. \tag{S-6}$$

We regard the variance V of \vec{x} as the output of this system. When all particles constitute a connected graph, the rank of L is N - 1 [1]. Note that

$$\mathbf{L}\vec{1} = \vec{0},\tag{S-7}$$

where $\vec{1} = [1, 1, ..., 1]^T$ and $\vec{0} = [0, 0, ..., 0]^T$. **L** is a real symmetric matrix. Thus, we can expand **L** as

$$\mathbf{L} = \sum_{i=1}^{N-1} \lambda_i \vec{u}_i \vec{u}_i^T, \tag{S-8}$$

where \vec{u}_i is an eigenvector of \mathbf{L} and λ_i is the eigenvalue corresponding to \vec{u}_i . Notably, $\vec{1} \perp \vec{u}_i$. We can not obtain the inverse of \mathbf{L} to solve Eq. (S-1) because \mathbf{L} is not full rank. Thus, we define a full-rank real symmetric matrix $\tilde{\mathbf{L}}$ by using a non-zero constant β :

$$\tilde{\mathbf{L}} = \mathbf{L} + \beta \mathbf{1},\tag{S-9}$$

where

$$\mathbf{1} = \vec{1}\vec{1}^T. \tag{S-10}$$

By using $\tilde{\mathbf{L}}$, we can obtain a solution of Eq. (S-6) by

$$\vec{x} = \tilde{\mathbf{L}}^{-1}\vec{b}.\tag{S-11}$$

By multiplying $\vec{1}$ from the left in Eq. (S-3), we see that this solution satisfies $\sum x_i = 0$. The output V can be derived as follows:

$$V = \frac{\vec{x} \cdot \vec{x}}{N} = \frac{1}{N} \vec{b}^T (\tilde{\mathbf{L}}^{-1})^T \tilde{\mathbf{L}}^{-1} \vec{b}$$
$$= \frac{1}{N} \vec{b}^T \tilde{\mathbf{L}}^{-1} \tilde{\mathbf{L}}^{-1} \vec{b}, \qquad (S-12)$$

because $\tilde{\mathbf{L}}^{-1}$ is also a symmetric matrix. In the following equations, we regard each coupling strength W_{ij} as a parameter. Because we have introduced the parameter β , the parameter sensitivity for β should also be taken into account. However V is independent of β because

$$\begin{aligned} \frac{\partial V}{\partial \beta} &= -\frac{1}{N} \vec{b}^T \tilde{\mathbf{L}}^{-1} \left(\frac{\partial \tilde{\mathbf{L}}}{\partial \beta} \tilde{\mathbf{L}}^{-1} + \tilde{\mathbf{L}}^{-1} \frac{\partial \tilde{\mathbf{L}}}{\partial \beta} \right) \tilde{\mathbf{L}}^{-1} \vec{b} \\ &= -\frac{1}{N} \vec{b}^T \tilde{\mathbf{L}}^{-1} \left(\mathbf{1} \tilde{\mathbf{L}}^{-1} + \tilde{\mathbf{L}}^{-1} \mathbf{1} \right) \tilde{\mathbf{L}}^{-1} \vec{b} \\ &= -\frac{1}{N} \vec{b}^T \tilde{\mathbf{L}}^{-1} \left(\frac{2N}{\beta} \mathbf{1} \right) \tilde{\mathbf{L}}^{-1} \vec{b} \\ &= -\frac{1}{N} \vec{b}^T \tilde{\mathbf{L}}^{-1} \frac{2N^2}{\beta^2} \mathbf{1} \vec{b} \\ &= -\frac{1}{N} \vec{b}^T \tilde{\mathbf{L}}^{-1} \frac{2N^2}{\beta^2} \vec{0} \\ &= 0, \end{aligned}$$
(S-13)

where we used

$$\frac{\partial \tilde{\mathbf{L}}^{-1}}{\partial \beta} = -\tilde{\mathbf{L}}^{-1} \frac{\partial \tilde{\mathbf{L}}}{\partial \beta} \tilde{\mathbf{L}}^{-1}, \qquad (S-14)$$

$$\frac{\partial \mathbf{L}}{\partial \beta} = \mathbf{1}, \tag{S-15}$$

$$\tilde{\mathbf{L}}^{-1} = \sum_{i=1}^{N-1} \frac{1}{\lambda_i} \vec{u}_i \vec{u}_i^T + \frac{1}{\beta} \mathbf{1}, \qquad (S-16)$$

$$\mathbf{1}\tilde{\mathbf{L}}^{-1} = \frac{N}{\beta}\mathbf{1}.$$
 (S-17)

The IMPS is derived as

$$IMPS = \sum_{\langle ij \rangle} \left| \frac{W_{ij}}{V} \frac{\partial V}{\partial W_{ij}} \right| + \left| \frac{\beta}{V} \frac{\partial V}{\partial \beta} \right|$$
$$= \frac{1}{N} \sum_{\langle ij \rangle} \left| \frac{W_{ij}}{V} \frac{\partial \vec{b}^T \tilde{\mathbf{L}}^{-1} \tilde{\mathbf{L}}^{-1} \vec{b}}{\partial W_{ij}} \right| + \frac{1}{N} \left| -\frac{\beta}{V} \vec{b}^T \tilde{\mathbf{L}}^{-1} \left(\mathbf{1} \tilde{\mathbf{L}}^{-1} + \tilde{\mathbf{L}}^{-1} \mathbf{1} \right) \tilde{\mathbf{L}}^{-1} \vec{b} \right|$$
$$= \frac{1}{N} \sum_{\langle ij \rangle} \left| -\frac{W_{ij}}{V} \vec{b}^T \tilde{\mathbf{L}}^{-1} \left(\frac{\partial \tilde{\mathbf{L}}}{\partial W_{ij}} \tilde{\mathbf{L}}^{-1} + \tilde{\mathbf{L}}^{-1} \frac{\partial \tilde{\mathbf{L}}}{\partial W_{ij}} \right) \tilde{\mathbf{L}}^{-1} \vec{b} \right|$$
$$+ \frac{1}{N} \left| -\frac{\beta}{V} \vec{b}^T \tilde{\mathbf{L}}^{-1} \left(\mathbf{1} \tilde{\mathbf{L}}^{-1} + \tilde{\mathbf{L}}^{-1} \mathbf{1} \right) \tilde{\mathbf{L}}^{-1} \vec{b} \right|, \qquad (S-18)$$

where $\langle \rangle$ is the summation over the pairs of (i, j) with $W_{ij} \neq 0$. Here we assume that SPSs have the same sign. By using

$$\sum_{\langle ij\rangle} W_{ij} \frac{\partial \tilde{\mathbf{L}}}{\partial W_{ij}} = \mathbf{L}, \qquad (S-19)$$

we obtain

$$IMPS = \frac{1}{N} \left| -\frac{1}{V} \vec{b}^{T} \tilde{\mathbf{L}}^{-1} [\mathbf{L}\tilde{\mathbf{L}}^{-1} + \tilde{\mathbf{L}}^{-1} \mathbf{L}] \tilde{\mathbf{L}}^{-1} \vec{b} \right|$$
$$- \frac{\beta}{V} \vec{b}^{T} \tilde{\mathbf{L}}^{-1} \left(\mathbf{1}\tilde{\mathbf{L}}^{-1} + \tilde{\mathbf{L}}^{-1} \mathbf{1} \right) \tilde{\mathbf{L}}^{-1} \vec{b} \right|$$
$$= \frac{1}{N} \left| -\frac{1}{V} \vec{b}^{T} \tilde{\mathbf{L}}^{-1} \left[(\mathbf{L} + \beta \mathbf{1}) \tilde{\mathbf{L}}^{-1} - \tilde{\mathbf{L}}^{-1} (\mathbf{L} + \beta \mathbf{1}) \right] \tilde{\mathbf{L}}^{-1} \vec{b} \right|$$
$$= \frac{1}{N} \left| -\frac{1}{V} \vec{b}^{T} \tilde{\mathbf{L}}^{-1} [\tilde{\mathbf{L}}\tilde{\mathbf{L}}^{-1} + \tilde{\mathbf{L}}^{-1} \tilde{\mathbf{L}}] \tilde{\mathbf{L}}^{-1} \vec{b} \right|$$
$$= \frac{1}{N} \left| -\frac{2}{V} \vec{b}^{T} \tilde{\mathbf{L}}^{-1} [\vec{\mathbf{L}}^{-1} \vec{b} \right|$$
$$= 2.$$
(S-20)

Analysis S2: Nonlinear Model

The dynamics of phase oscillators are expressed as

$$\frac{d\theta_i}{dt} = \omega_i + \sum_{j=1}^N K_{ij} \sin(\theta_j - \theta_i), \qquad (S-21)$$

where ω_i is the natural frequency of oscillator *i*, **K** is the symmetric connection weight matrix and $K_{ij} \geq 0$. We use the circular variance V_c of the oscillators [2]

$$V_c = 1 - r = 1 - \frac{1}{N}\sqrt{C^2 + S^2}$$
(S-22)

in the phase-locked state as the output, where r is the Kuramoto order parameter, $C = \sum_{i=1}^{N} \cos \theta_i$ and $S = \sum_{i=1}^{N} \sin \theta_i$. We can assume $\sum_{i=1}^{N} \omega_i = 0$ without loss of generality. In the phase-locked state, the right-hand side y'_i of Eq. (S-21) is 0; i.e.,

$$\vec{y'} = \vec{0}.\tag{S-23}$$

Here we derive the relationship between the connection weights and the phases under the condition that Eq. (S-23) is satisfied. For a small change $\Delta \vec{\theta}$ of $\vec{\theta}$, we denote the resulting small change in **K** by $\Delta \mathbf{K}$. We obtain

$$y'_{i} + \Delta y'_{i} = \omega_{i} + \sum_{j=1}^{N} (K_{ij} + \Delta K_{ij}) \sin(\theta_{j} + \Delta \theta_{j} - \theta_{i} - \Delta \theta_{i})$$

$$\approx \omega_{i} + \sum_{j=1}^{N} (K_{ij} + \Delta K_{ij}) \left[\sin(\theta_{j} - \theta_{i}) + \cos(\theta_{j} - \theta_{i}) (\Delta \theta_{j} - \Delta \theta_{i}) \right].$$
(S-24)

Subtracting y'_i from both sides yields

$$\Delta y'_{i} \approx \sum_{j=1}^{N} K_{ij} \cos(\theta_{j} - \theta_{i}) (\Delta \theta_{j} - \Delta \theta_{i}) + \sum_{j=1}^{N} \Delta K_{ij} \left[\sin(\theta_{j} - \theta_{i}) + \cos(\theta_{j} - \theta_{i}) (\Delta \theta_{j} - \Delta \theta_{i}) \right].$$
(S-25)

Thus, we obtain

$$\frac{\partial y'_i}{\partial \theta_j} = J_{ij}, \tag{S-26}$$

$$\frac{\partial y'_i}{\partial K_{lm}} = \begin{cases} \sin(\theta_m - \theta_l) & i = l \\ 0 & i \neq l \end{cases},$$
(S-27)

where

$$J_{ij} = \begin{cases} -\sum_{s=1}^{N} K_{is} \cos(\theta_s - \theta_i) & i = j \\ K_{ij} \cos(\theta_j - \theta_i) & i \neq j \end{cases}.$$
 (S-28)

Adding the same value to all θ s of a phase-locked solution results in another phase-locked solution, and the latter cannot be distinguished from the former in terms of the circular variance V_c . Thus, we cannot determine the unique phase-locked solution for this model. However, we can set the average phase to 0, which will not ruin the generality of our argument. By assuming $\sum_{i=1}^{N} \theta_i = 0$, we can replace Eq. (S-23) with

$$y_i \equiv \omega_i + \sum_{j=1}^N K_{ij} \sin(\theta_j - \theta_i) - \sum_{j=1}^N \theta_j = 0.$$
 (S-29)

Hence, $\partial y_i / \partial \theta_j$ can be derived as

$$\frac{\partial y_i}{\partial \theta_j} = J_{ij} - 1 \equiv \tilde{J}_{ij}. \tag{S-30}$$

The matrix $\tilde{\mathbf{J}} = (\tilde{J}_{ij})$ is full rank. Thus, we have

$$\frac{\partial \theta_i}{\partial K_{lm}} = -\sum_{j=1}^N (\tilde{\mathbf{J}}^{-1})_{ij} \delta_{jl} \sin(\theta_m - \theta_l)$$
$$= -(\tilde{\mathbf{J}}^{-1})_{il} \sin(\theta_m - \theta_l).$$
(S-31)

Hence, the derivative of V_c with respect to K_{lm} is given by

$$\frac{\partial V_c}{\partial K_{lm}} = -\frac{1}{2N} \left(C^2 + S^2 \right)^{-1/2} \frac{\partial \left[\left(\sum_{i=1}^N \cos \theta_i \right)^2 + \left(\sum_{i=1}^N \sin \theta_i \right)^2 \right]}{\partial K_{lm}} \\
= \frac{-1}{N^2 r} \left(-C \sum_{i=1}^N \sin \theta_i \frac{\partial \theta_i}{\partial K_{lm}} + S \sum_{i=1}^N \cos \theta_i \frac{\partial \theta_i}{\partial K_{lm}} \right) \\
= \frac{1}{N^2 r} \left(S \sum_{i=1}^N \cos \theta_i (\tilde{\mathbf{J}}^{-1})_{il} - C \sum_{i=1}^N \sin \theta_i (\tilde{\mathbf{J}}^{-1})_{il} \right) \sin(\theta_m - \theta_l).$$
(S-32)

From the above analysis, we numerically obtain the IMPS by using

$$IMPS = \sum_{\langle lm \rangle} |SPS_{lm}|$$
$$= \sum_{\langle lm \rangle} \left| \frac{K_{lm}}{V_c} \frac{\partial V_c}{\partial K_{lm}} \right|, \qquad (S-33)$$

where $\langle \rangle$ is the summation over the pairs of (l, m) with $K_{lm} \neq 0$.

Analysis S3: Phase Oscillators on Path Graph

In general, nonlinearly coupled oscillator models can not be solved analytically. However, a solution can be obtained as follows for phase oscillators on a path graph. Here, we assume N oscillators are located on a path graph (Fig. 5B). Thus, on a path graph, N-2 vertices are of degree 2, and 2 vertices are of degree 1. We assume that $-\omega_1 = \omega_N = 1$ and $\omega_i = 0$ for 1 < i < N. Under these assumptions, the dynamics are given by

$$\dot{\theta}_{1} = -1 + \alpha \sin(\theta_{2} - \theta_{1}),
\dot{\theta}_{2} = \alpha \sin(\theta_{3} - \theta_{2}) + \alpha \sin(\theta_{1} - \theta_{2}),
\vdots
\dot{\theta}_{N-1} = \alpha \sin(\theta_{N} - \theta_{N-1}) + \alpha \sin(\theta_{N-2} - \theta_{N-1}),
\dot{\theta}_{N} = 1 + \alpha \sin(\theta_{N-1} - \theta_{N}),$$
(S-34)

where α is the coupling strength. Thus, all of N oscillators are spaced at regular intervals in the phaselocked state. N oscillators are located in a line every other $\Delta \theta = \sin^{-1}(1/\alpha) > 0$. We can assume $\theta_i = (i-1)\Delta\theta$ in the phase-locked state without loss of generality. The circular variance V_c is given by

$$V_c = 1 - r = 1 - \frac{1}{N} \left| \sum_{s=1}^{N} e^{i(s-1)\Delta\theta} \right|.$$
 (S-35)

 ${\bf J},$ which is defined in Supplemental Materials Analysis S2, is expressed as

$$\mathbf{J} = \alpha \cos(\Delta \theta) \begin{pmatrix} -1 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & & 0 \\ \vdots & \vdots & & \ddots & \vdots \\ 0 & 0 & 0 & \cdots & -1 \end{pmatrix}.$$
 (S-36)

The IMPS of this undirectional model is obtained by using

IMPS =
$$\frac{\alpha}{V_c} \sum_{\langle lm \rangle} \left| \frac{\partial V_c}{\partial K_{lm}} + \frac{\partial V_c}{\partial K_{ml}} \right|$$

= $\frac{\alpha \sin(\Delta \theta)}{V_c N^2 r} \sum_{n=1}^{N-1} |S\kappa_n^c - C\kappa_n^s - S\kappa_{n+1}^c + C\kappa_{n+1}^s|,$ (S-37)

where

$$\sum_{n=1}^{N} (\mathbf{J})_{in} \kappa_n^c = \cos \theta_i, \tag{S-38}$$

$$\sum_{n=1}^{N} (\mathbf{J})_{in} \kappa_n^s = \sin \theta_i.$$
(S-39)

Since **J** is of rank N-1 [1], κ_i^s and κ_i^c have uncertainty. Thus, we assume that $\kappa_1^s = \kappa_1^c = 0$ and determine κ_n^s and κ_n^c by recursively using κ_i^s (i < n) to obtain

$$\kappa_n^c = \frac{1}{\alpha \cos(\Delta \theta)} \sum_{s=1}^{n-1} (n-s) \cos[(s-1)\Delta \theta]$$

$$= \frac{1}{\alpha \cos(\Delta \theta)} \operatorname{Re} \left[n \frac{z^{n-1}-1}{z-1} - \left(\frac{z^n-z}{z-1}\right)' \right]$$

$$\kappa_n^s = \frac{1}{\alpha \cos(\Delta \theta)} \sum_{s=1}^{n-1} (n-s) \sin[(s-1)\Delta \theta]$$

$$= \frac{1}{\alpha \cos(\Delta \theta)} \operatorname{Im} \left[n \frac{z^{n-1}-1}{z-1} - \left(\frac{z^n-z}{z-1}\right)' \right]$$
(S-40)

where

$$z = \cos(\Delta\theta) + i\sin(\Delta\theta). \tag{S-41}$$

Thus, assuming $N\Delta\theta \leq 2\pi$, IMPS is derived as

$$IMPS = \frac{\alpha \sin(\Delta \theta)}{V_c N^2 r \alpha \cos(\Delta \theta)} \sum_{n=1}^{N-1} |SRe[f_n(z)] - CIm[f_n(z)] - SRe[f_{n+1}(z)] + CIm[f_{n+1}(z)]|$$

$$= \frac{\tan(\Delta \theta)}{V_c N^2 r} \sum_{n=1}^{N-1} |SRe[f_n(z) - f_{n+1}(z)] - CIm[f_n(z) - f_{n+1}(z)]|$$

$$= \frac{\tan(\Delta \theta)}{V_c N^2 r} \sum_{n=1}^{N-1} \left| Im \left(\frac{z^N - 1}{z - 1} \overline{[f_n(z) - f_{n+1}(z)]} \right) \right|$$

$$= \frac{\tan(\Delta \theta)}{V_c N^2 r} \left| Im \left[\frac{z^N - 1}{z - 1} \overline{\left(\sum_{n=1}^{N-1} \frac{-z^n + 1}{z - 1} \right)} \right] \right|$$

$$= \frac{\tan(\Delta \theta)}{N^2 r (1 - r)} \left| Im \left[\frac{z^N - 1}{z - 1} \overline{\left(\frac{-z^N + N(z - 1) + 1}{(z - 1)^2} \right)} \right] \right|, \quad (S-42)$$

where we have used

$$f_{n}(z) = n \frac{z^{n-1} - 1}{z - 1} - \left(\frac{z^{n} - z}{z - 1}\right)', \qquad (S-43)$$

$$f_{n}(z) - f_{n+1}(z) = n \frac{z^{n-1} - 1}{z - 1} - \left(\frac{z^{n} - z}{z - 1}\right)' - (n + 1)\frac{z^{n} - 1}{z - 1} + \left(\frac{z^{n+1} - z}{z - 1}\right)'$$

$$= n \frac{z^{n-1} - z^{n}}{z - 1} - \frac{z^{n} - 1}{z - 1} - \left(\frac{z^{n} - z}{z - 1} - \frac{z^{n+1} - z}{z - 1}\right)'$$

$$= -nz^{n-1} - \frac{z^{n} - 1}{z - 1} + nz^{n-1}$$

$$= -\frac{z^{n} - 1}{z - 1}. \qquad (S-44)$$

Figure S1: Correlation between IMPS and Average Path Length



Figure S1. (A) Scatter diagram of $\text{IMPS}(\alpha = 10) - \text{IMPS}(\alpha = 100)$ against average path length for 50 Watts–Strogatz networks (N = 1000, rewiring probability= 0.05). Correlation coefficient r is -0.43 (p < 0.01). (B) Scatter diagram of $\text{IMPS}(\alpha = 2.5) - \text{IMPS}(\alpha = 100)$ against average path length for 50 Barabási–Albert networks (N = 1000). Correlation coefficient r is 0.0068 (non-significant).

References

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- 2. N. I. Fisher: Statistical Analysis of Circular Data (Cambridge University Press, 1995).