Jacobian geometry

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(Dated: February 4, 2022)

The Jacobian distance aims to be a generalization of the diffusion distance, thus allowing us to define and exploit an underlying geometry with a metric distance based on the signal propagation of a general dynamical process, instead of being limited to the random walk, diffusive dynamics. Therefore, we want to shed light on the implications of such a dynamically-induced geometry and what are its advantages (and limitations) when compared to more classical network geometries. On the other hand, and similarly to the diffusion distance, we aim to unveil network properties that remain hidden if one uses a purely topological description, such as the presence of functional clusters or other mesoscale organization.

In this document we introduce the definition of the Jacobian distance, and we briefly comment its similarities and differences with other distances defined on complex networks. We present a bunch of dynamical models for which the Jacobian distance are calculated analytically and compared with simulations.

I. ANALYTICAL DERIVATION OF THE JACOBIAN DISTANCE

Let us consider a networked dynamical system $\dot{x}_k = f_k(x_1,\dots,x_N) \equiv f_k(\mathbf{x})$, where $x_k(t)$ is a variable representing the state of node k at time t. The steady state of the dynamical system is given by $f_k(\mathbf{x}^*)=0$. Assume this state is slightly perturbed such that $x_i^* \to x_i^* + \mathrm{d}x_i$ and $x_j^* \to x_j^* + \mathrm{d}x_j$, with $|\,\mathrm{d}x_i|$ and $|\,\mathrm{d}x_i| \ll 1$. The vector fields evaluated at the perturbed steady-state can be written as

$$\begin{aligned}\widetilde{f}_k(i,j) &\equiv f_k(x_1^*,\dots,x_i^*+\mathrm{d}x_i,\dots,x_j^*+\mathrm{d}x_j,\dots x_N^*)\\ &\approx \left.\frac{\partial f_k}{\partial x_i}\right|_{\mathbf{x}^*}\mathrm{d}x_i + \left.\frac{\partial f_k}{\partial x_j}\right|_{\mathbf{x}^*}\mathrm{d}x_j. \end{aligned} \tag{1}$$

In matricial form we can write $\widetilde{\mathbf{f}}(i,j) \approx \widehat{J}(\mathbf{x}^*)\,\mathrm{d}\mathbf{x}(i,j)$, where $\widehat{J}(\mathbf{x}^*)$ is the Jacobian matrix evaluated at the steady state and $\mathrm{d}\mathbf{x}(i,j) = (0,\dots\mathrm{d}x_i,\dots,\mathrm{d}x_j,\dots,0)^T$ is the vector with the intensity of the perturbed variables. Note that simultaneous perturbations in $n \leq N$ variables can be expressed with the same equation, just by changing the number of arguments.

If we perturb with respect to a single variable i we can write $\widetilde{\mathbf{f}}(i) = \widehat{J}(\mathbf{x}^*)\,\mathrm{d}x_i\mathbf{e}_{(i)}$, where $\mathbf{e}_{(i)}$ is the unitary vector in the i-direction. The difference between states is

$$d_{ij}^2 = \|\widetilde{\mathbf{f}}(i) - \widetilde{\mathbf{f}}(j)\|^2 = \|\widehat{J}(\mathbf{x}^*)(\mathbf{e}_{(i)}\,\mathrm{d}x_i - \mathbf{e}_{(j)}\,\mathrm{d}x_j)\|^2, \tag{2}$$

and if we take the perturbation intensity as the same, $\mathrm{d}x_i = \mathrm{d}x_j = \epsilon$, this simplifies to

$$d_{ij}^2(\epsilon) = \|\widehat{J}(\mathbf{x}^*)(\mathbf{e}_{(i)} - \mathbf{e}_{(j)})\|^2\epsilon^2. \tag{3}$$

In general we have that $\|\mathbf{u}-\mathbf{v}\|^2 = \|\mathbf{u}\|^2 + \|\mathbf{v}\|^2 - \mathbf{v}\mathbf{u}^T - \mathbf{u}\mathbf{v}^T$. Expanding accordingly Eq. (3), we obtain

$$\begin{aligned} d_{ij}^2\epsilon^{-2} &= \|\widehat{J}(\mathbf{x}^*)\mathbf{e}_{(i)}\|^2 + \|\widehat{J}(\mathbf{x}^*)\mathbf{e}_{(j)}\|^2\\ &\quad - [\widehat{J}(\mathbf{x}^*)\mathbf{e}_{(i)}][\mathbf{e}_{(j)}^T\widehat{J}(\mathbf{x}^*)^T] - [\widehat{J}(\mathbf{x}^*)\mathbf{e}_{(j)}][\mathbf{e}_{(i)}^T\widehat{J}(\mathbf{x}^*)^T]\\ &= \|\widehat{J}^*_{(i)}\|^2 + \|\widehat{J}^*_{(j)}\|^2 - \widehat{J}^*_{(i)}\widehat{J}^*_{(j)}{}^T - \widehat{J}^*_{(j)}\widehat{J}^*_{(i)}{}^T, \end{aligned} \tag{4}$$

where $\widehat{J}^*_{(i)}$ is the ith column of the Jacobian evaluated at the steady state.

The same procedure can be applied taking into account the time evolution of the perturbation. Let us write $x_k(t) = x_k^* + \delta x_k(t)$, therefore

$$\dot{x}_k(t) = \delta\dot{x}_k(t) = f_k(\mathbf{x}^*+\delta\mathbf{x}(t)) = \sum_{i=1}^{N}\left.\frac{\partial f_k}{\partial x_i}\right|_{\mathbf{x}^*}\delta x_i(t) + \mathcal{O}(\delta\mathbf{x}^2(t)). \tag{5}$$

Matricially we have that $\delta\dot{\mathbf{x}} \approx \widehat{J}(\mathbf{x}^*)\delta\mathbf{x}(t)$, whose solution is $\delta\mathbf{x}(t) = e^{\widehat{J}(\mathbf{x}^*)t}\delta\mathbf{x}(0)$. If initially it is the node k that is perturbed, we have that $\delta\mathbf{x}(0) = \mathrm{d}x_k\mathbf{e}_{(k)}$, then we write $\delta\mathbf{x}_{(k)}(t) \equiv e^{\widehat{J}(\mathbf{x}^*)t}\,\mathrm{d}x_k\mathbf{e}_{(k)}$. The Jacobian distance is defined as the time evolution of the difference between two perturbations initially placed in nodes i and j

$$\delta_{ij}^2(\tau) = \|\delta_{(i)}\mathbf{x}(t) - \delta_{(j)}\mathbf{x}(t)\|^2 \tag{6}$$

$$= \|e^{\widehat{J}(\mathbf{x}^*)\tau}[\mathrm{d}x_i\mathbf{e}_{(i)} - \mathrm{d}x_j\mathbf{e}_{(j)}]\|^2 \tag{7}$$

The diffusion distance has the same form as Eq. (7) but with the Jacobian instead of the Laplacian in the argument of the exponential [1]. Therefore the Jacobian distance somehow generalizes the diffusion distance for dynamics that are not purely diffusive.

A. Mean-field Jacobian distance

No assumptions have been made on the vector fields $f_k(\mathbf{x})$ to derive the Jacobian distance. Indeed, Eq. (7) is the most general expression, but it is difficult to find how it depends on the network properties, for example, how

d_{ij} depends on k_i and k_j. If we make some assumptions, Eq. (7) can be simplified and maybe this can lead us to find such dependencies. Here there is a try.

Let us take the vector fields to be separable *a la* Barzel

$$f_i(\mathbf{x}) = F(x_i) + \sum_{j=1}^{N} A_{ij} G(x_i, x_j). \tag{8}$$

In [2] it is found that an N-dimensional dynamical system with vector field of the form (8) can be rewritten as a one-dimensional system

$$\dot{x}_{\text{eff}}(t) = F(x_{\text{eff}}) + \beta_{\text{eff}} G(x_{\text{eff}}, x_{\text{eff}}), \tag{9}$$

with

$$x_{\text{eff}} = \frac{\langle s^{\text{out}} x \rangle}{\langle s \rangle}. \tag{10}$$

The interaction term is multiplied by a constant which only depends on the topology of the network, $\beta_{\text{eff}} = \langle s^{\text{out}} s^{\text{in}} \rangle / \langle s \rangle$, where s^{in} and s^{out} are the vectors of ingoing and outgoing weighted degrees, respectively $(s_1^{\text{in}}, \ldots, s_N^{\text{in}})^\intercal$ and $(s_1^{\text{out}}, \ldots, s_N^{\text{out}})^\intercal$. If the network is undirected and unweighted, we obtain

$$\beta_{\text{eff}} = \frac{\langle k^2 \rangle}{\langle k \rangle}. \tag{11}$$

In summary, the fixed points of the original system will depend on the entire adjacency matrix plus the parameters of the functions $F(\cdot)$ and $G(\cdot, \cdot)$, hence being quite difficult to analyse. We can create, though, a mapping to a situation in which the fixed points of a new variable x_{eff} have all the dependency on the network topology inside β_{eff}, hence clearly separating the contributions of the topology and the dynamics.

The fixed points of the original system, the ones around which we perturb to find the time evolution of the Jacobian variable, are given by

$$F(x_i^*) + \sum_{j=1}^{N} A_{ij} G(x_i^*, x_j^*) = 0. \tag{12}$$

A mean-field approximation can be used if we substitute $x_j^* \to x_{\text{eff}}^*$ in this last equation, yielding

$$F(x_i^*) + k_i G(x_i^*, x_{\text{eff}}^*) = 0. \tag{13}$$

So we can write in a closed form x_i^* in terms of the degree of node i, x_{eff}, and the parameters of the dynamical model encoded in $F(\cdot)$ and $G(\cdot, \cdot)$. This mean-field critical point could be inserted in the expression of the Jacobian distance Eq. (7), when evaluating the Jacobian at the steady-state, and maybe things simplify somehow. Haven't tried yet to go further...

II. ANALOGIES AND DIFFERENCES BETWEEN JACOBIAN DISTANCE AND OTHER DISTANCES

A. Brockmann distance [3]

It is computed from purely topological information and no dynamics are involved: we just need a quantity associated to each link (e.g., flows), that define the link distance, and Brockamnn's effective distance between two nodes is just the sum of these link distances along the path that gives the lowest value. On the contrary, the Jacobian distance is intimately related to a certain dynamics and it takes into account the (weighted) contribution of all the paths between the nodes.

B. Barzel-like distances [4–7]

Many (all?) of Barzel's metrics are based in perturbations to one node, while the Jacobian distance is computed from the simultaneous perturbation of two nodes (could we generalize it and use a group of nodes larger than 2, kind of Jacobian distance for hypergraphs? Probbly yes). Moreover, Barzel's framework is based on constant, time-independent perturbations, while in Jacobian distance the perturbations are instantaneous, Dirac-like. In other words, for Barzel, after perturbing $x_i \to x_i + \mathrm{d}x_i$, node i stays fixed at $x_i + \mathrm{d}x_i$), while for us the perturbations are instantaneous and time-dependent, so the perturbed node relaxes to a state different than $x_i + \mathrm{d}x_i$.

C. Diffusion distance [1]

The computation of the diffusion distance is based on the graph Laplacian, therefore it is only meaningful for diffusive dynamics, or diffusive approximations to non-diffusive dynamics, e.g., Kuramoto's $\sin(\theta_i - \theta_j) \approx \theta_i - \theta_j$. The diffusion distance, moreover, has a clear physical interpretation in terms of random walkers propagation and encountering across the network. For the Jacobian distance, the analogy is perturbation signals travelling and interfering between them. The diffusion distance $d_{ij}(\tau)$ between nodes i and j is low when two walkers starting simultaneously at both nodes have a high chance of meeting at time τ at the same nodes, not necessarily i and j, which in general occurs when i and j are connected by many different paths. This point of view is also valid for the Jacobian distance: it takes its largest value for small times because the perturbations are localized in i and j and have barely propagated, and it decays in time, decaying faster for nodes that are close in the *Jacobian space* which in general will be those that are connected by many paths.

III. DYNAMICS TO TEST IN THE JACOBIAN DISTANCE

A. Biochemical dynamics (Mass-action kinetics)

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = F - Bx_i - R\sum_{j=1}^{N} A_{ij}x_i x_j,$$

whose Jacobian $\frac{\partial f_i}{\partial x_k}$ is

$$-B\delta_{ik} - R\left[\delta_{ik}\sum_j A_{ij}x_j + (1-\delta_{ik})A_{ij}x_i\right].$$

B. Birth-death processes (Population dynamics)

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = -Bx_i^b + R\sum_{j=1}^{N} A_{ij}x_j^a,$$

whose Jacobian $\frac{\partial f_i}{\partial x_k}$ is

$$-Bbx_i^{b-1}\delta_{ik} + RaA_{ik}x_k^{a-1}.$$

In [4] it is used $b = 2, a = 1$. In [7] it is used $b = 3, a = 2$. In [6] it is used $b = 1/2, a = 0.2$.

C. Regulatory dynamics (Michaelis-Menten equation)

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = -Bx_i^a + R\sum_{j=1}^{N} A_{ij}\frac{x_j^h}{1+x_j^h},$$

whose Jacobian $\frac{\partial f_i}{\partial x_k}$ is

$$-Bax_i^{a-1}\delta_{ik} + RA_{ik}\frac{hx_k^{h-1}}{(1+x_k^h)^2}.$$

In [4] it is used $a = 1, h = 1$. In [5] it is used $a = 1/2, h = 1/3$. In [6] it is used $a = 0.4, h = 0.2$. In [7] it is used $a = 1, h = 1/3$ and $a = 1, h = 2$.

D. Epidemics dynamics (SIS model)

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = -Bx_i - R\sum_{j=1}^{N} A_{ij}(1-x_i)x_j,$$

whose Jacobian $\frac{\partial f_i}{\partial x_k}$ is

$$-B\delta_{ik} + R\left[(1-\delta_{ik})A_{ik}(1-x_i) - \delta_{ik}\sum_j A_{ij}x_j\right].$$

E. Synchronization dynamics (Kuramoto model) [Not used by Barzel]

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = \omega_i + R\sum_{j=1}^{N} A_{ij}\sin(x_j - x_i),$$

whose Jacobian $\frac{\partial f_i}{\partial x_k}$ is

$$-R\delta_{ik}\sum_{j(\neq i)} A_{ij}\cos(x_j - x_i) + (1-\delta_{ik})RA_{ik}\cos(x_k - x_i)$$

F. Mutualistic dynamics

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = x_i(1-x_i) + R\sum_{j=1}^{N} A_{ij}x_i\frac{x_j^b}{1+x_j^b},$$

whose Jacobian $\frac{\partial f_i}{\partial x_k}$ is

$$B(1-2x_i)\delta_{ik} + R\left[\delta_{ik}\sum_j A_{ij}\frac{x_j^b}{1+x_j^b} + (1-\delta_{ik})A_{ik}x_i\frac{bx_k^{b-1}}{(1+x_k^b)^2}\right].$$

In [7] it is used $b = 1$. In [6] it is used $b = 2$.

G. Neuronal dynamics

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = -Bx_i + C\tanh x_i + R\sum_{j=1}^{N} A_{ij}\tanh x_j,$$

whose Jacobian $\frac{\partial f_i}{\partial x_k}$ is

$$\left[-B + C\,\mathrm{sech}^2(x_i)\right]\delta_{ik} + RA_{ik}\,\mathrm{sech}^2(x_k).$$

H. Noisy voter model [not used by Barzel]

$$\frac{\mathrm{d}x_i}{\mathrm{d}t} = A - Bx_i + \frac{C}{k_i}\sum_{j=1}^{N} A_{ij}x_j,$$

whose Jacobian is

$$\delta_{ik}\left(-B+\frac{C}{k_i}A_{ik}\right)+(1-\delta_{ik})\frac{C}{k_i}A_{ik}$$

IV. SIMULATIONS

For several of the above dynamics, we compute the Jacobian distance in two different ways: *(i)* directly employing the analytical expression of the Jacobian in Eq. (7), and *(ii)* integrating the dynamical equations up to the steady state and then perturb it in order to follow the temporal evolution as in Eq. (6). A third option that we have not yet explored would be to directly simulate the dynamics under consideration, in the same way we simulate in the diffusion distance the actual walkers crossing the network. This third option would be very convenient to scale up to large networks, since method *(ii)* integrates an $N \times N$ system of equations, which becomes prohibitively slow for networks of few hundreds of nodes. For method *(i)*, it would be nice to find a way to obtain a simpler analytical expression for the Jacobian distance, via e.g., the mean-field Jacobian distance or by substituting the adjacency matrix elements by an annealed approximation $A_{ij} = k_i k_j/(N\langle k\rangle)$.

The behavior of the mean Jacobian distance is shown in Fig. 1. The two types of curves, $\delta(\tau) \sim 0.07$ and $\delta(\tau) \sim 0.7$ are consequence of the strength of the perturbation applied, which are the same for each group of curves. Indeed, when $\tau \sim 0$, the diffusion distance only depends on the perturbation strength. For large τ, the mean Jacobian distance tends to 0, as one would expect by looking at Eq. (7). We could compare the mean Jacobian distance with the Jacobian distance $\delta_{ij}(\tau)$ for different choices of nodes i and j: for example how $\delta_{ij}(\tau)$ depends on the (link) distance between i and j, how $\delta_{ij}(\tau)$ depends on the degrees of i and j, etc.

In the Videos folder (see left bar in the Overleaf menu) we show a video of the behavior of $\delta_{ij}(\tau)$. No clear patterns arise, the only thing it seems significant is that for low degree nodes the Jacobian distance decays slower (see a snapshot of this in Fig. 2).

To shed light on the role played by the topology, we simulate the process in a network in a stochastic block model. The Jacobian distance at some intermediate time is shown in Fig. 3, and the full video can be found in the Videos/ folder. It does not seem that the SIS model feel the communities, but this might be have its origin in the model itself, so other models would feel them, or could be that the chosen parameters of the block model are not appropiate. This needs further exploration.

[1] M. De Domenico, Diffusion geometry unravels the emergence of functional clusters in collective phenomena, Physical Review Letters **118**, 168301 (2017).

[2] J. Gao, B. Barzel, and A.-L. Barabási, Universal resilience patterns in complex networks, Nature **530**, 307 (2016).

[3] D. Brockmann and D. Helbing, The hidden geometry of complex, network-driven contagion phenomena, science **342**, 1337 (2013).

[4] B. Barzel and A.-L. Barabási, Universality in network dynamics, Nature Physics **9**, 673 (2013).

[5] B. Barzel, Y.-Y. Liu, and A.-L. Barabási, Constructing minimal models for complex system dynamics, Nature Communications **6**, 1 (2015).

[6] C. Hens, U. Harush, S. Haber, R. Cohen, and B. Barzel, Spatiotemporal signal propagation in complex networks, Nature Physics **15**, 403 (2019).

[7] U. Harush and B. Barzel, Dynamic patterns of information flow in complex networks, Nature Communications **8**, 1 (2017).

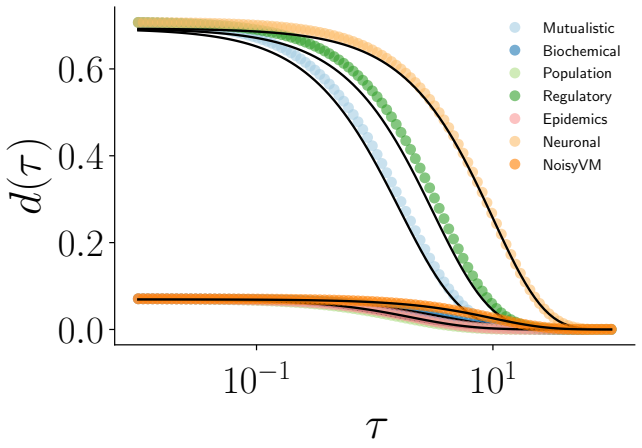

FIG. 1. Average Jacobian distance in Erdos-Renyi networks with $N = 50$ and $\langle k \rangle = 5$. We verify that the network form a single connected component. The top curves have an unbounded domain in their state variable $x(t)$ so the perturbation strength is 0.5. The bottom curves have a bounded state variable $0 < x(t) < 1$ so the perturbation strength has been chosen smaller, 0.05. For the simulations, we consider in all cases a random initial condition where $x_i(0) \in \mathcal{U}(0, 1)$.

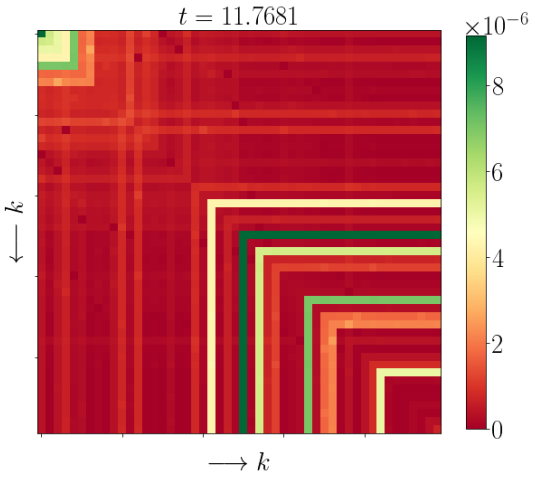

FIG. 2. Jacobian distance in Erdos-Renyi networks with $N = 50$ and $\langle k \rangle = 5$. Simulated for an SIS model, where the dynamical equations are integrated. We verify that the network form a single connected component. The node degrees are sorted from lowest to highest. The full video is in Videos/ folder.

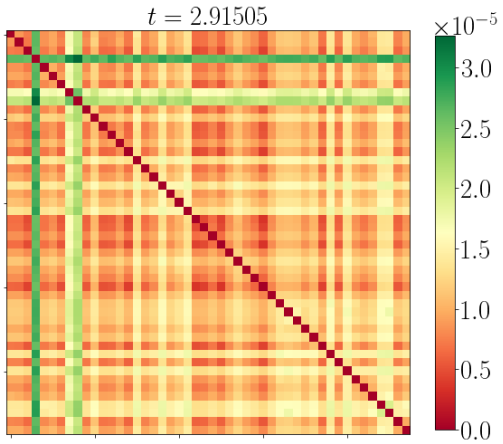

FIG. 3. Jacobian distance for a Stochastic Block Model with 3 communities, 16 nodes per community, an average degree 6 and a fixed average out-degree 0.1. Simulated for an SIS model, where the dynamical equations are integrated. We verify that the network form a single connected component. The full video is in Videos/ folder.