Laplacian renormalization group for heterogeneous networks

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The renormalization group is the cornerstone of the modern theory of universality and phase transitions and it is a powerful tool to scrutinize symmetries and organizational scales in dynamical systems. However, its application to complex networks has proven particularly challenging, owing to correlations between intertwined scales. To date, existing approaches have been based on hidden geometries hypotheses, which rely on the embedding of complex networks into underlying hidden metric spaces. Here we propose a Laplacian renormalization group diffusion-based picture for complex networks, which is able to identify proper spatiotemporal scales in heterogeneous networks. In analogy with real-space renormalization group procedures, we first introduce the concept of Kadanoff supernodes as block nodes across multiple scales, which helps to overcome detrimental small-world effects that are responsible for cross-scale correlations. We then rigorously define the momentum space procedure to progressively integrate out fast diffusion modes and generate coarse-grained graphs. We validate the method through application to several real-world networks, demonstrating its ability to perform network reduction keeping crucial properties of the systems intact.

A basic open question in statistical physics of networks is how to define a reduction scheme to detect all internal characteristic scales that significantly exceed the microscopic one. This is the hunting ground for a very powerful tool in modern theoretical physics, the renormalization group (RG). The RG provides an elegant and precise theory of criticality and allows for connecting—via the scaling hypothesis—extremely varied spatiotemporal scales and understanding the fundamental concept of scale invariance. The formulation of the RG in complex networks is still an open issue. Different schemes have been introduced, such as spectral coarse-graining or box-covering methods, allowing the identification of general sets of scaling relations in networks, starting from the general assumption of fractality of the system. Nevertheless, small-world effects reflected in short path lengths overcomplicate the identification of ‘block nodes’, while Kadanoff’s decimation presents different issues when applied to real networks.

Solid efforts in the complex network community have been made to develop further RG techniques. In a pioneering work, García-Pérez et al. defined a geometric RG approach by embedding complex networks into underlying hidden metric geometrical spaces. This approach has found particular application in the RG analysis of the Human Connectome, by studying zoomed-out layers and evidencing self-similarity under particular coarse-graining transformations. Notwithstanding the power of these procedures, they all rely on the critical assumption that they dwell in different isomorphic geometric spaces, or consider a fitness distance between nodes, conditioning the probability of connection among nodes to establish subsequent supernodes. For example, these techniques may lead to...
Fourier space, and automatically induces a definition of coarse-grained scales and connections, and a renormalized ‘slow’ Laplacian on the coarse-grained graph. Finally, we apply the LRG to several actual networks, connecting the specific heat with the scale-invariant properties of a network, and show the ability of the method to perform network reduction and to capture essential properties of several systems.

Statistical physics of information network diffusion

Information communicability in complex networks is governed by the Laplacian matrix\(^{24,28}\), \(\mathbf{L}\), defined for undirected networks as \(L_{ij} = (\delta_{ij} - A_{ij})\), where \(A_{ij}\) are the elements of the adjacency matrix \(\mathbf{A}\) and \(\delta_{ij}\) is the Kronecker delta function. The evolution of information of a given initial specific state of the network, \(\mathbf{s}(0)\), will evolve with time, \(t\), as \(\mathbf{s}(t) = e^{-t\mathbf{L}}\mathbf{s}(0)\). The network propagator, \(\hat{K} = e^{-t\mathbf{L}}\), represents the discrete counterpart of the path-integral formulation of general diffusion processes\(^{20,30}\), and each matrix element \(K_{ij}\) describes the sum of diffusion trajectories along all possible paths connecting nodes \(i\) and \(j\) at time \(t\) (refs. 31–33). We assume connected networks to fulfill the ergodic hypothesis.

In terms of the network propagator (Methods), \(\hat{K}\), it is possible to define the ensemble of accessible information diffusion states\(^{25,26,34}\), namely,

\[
\hat{\rho}(t) = \frac{\hat{K}}{\text{Tr}(\hat{K})} = e^{-t\mathbf{L}}/\text{Tr}(e^{-t\mathbf{L}}),
\]

where \(\rho(t)\) is tantamount to the canonical density operator in statistical physics (or to the functional over fields configurations)\(^{33,36}\). It follows that \(\mathcal{S}(\rho(t))\) corresponds to the canonical system entropy\(^{20,26}\),

\[
\mathcal{S}(\rho(t)) = -\frac{1}{\log(N)} \sum_{\mu=1}^{N} \mu_i(t) \log \mu_i(t).
\]

where \(N\) is the number of network nodes, and \(\mu_i\) represents the specific \(\rho_i(t)\) set of eigenvalues. In particular, \(S \in [0,1]\) reflects the emergence of entropic transitions (or information propagation transitions, that is, diffusion) over the network\(^{26}\). By increasing the diffusion time \(t\) from \(0\) to \(\infty\), \(\mathcal{S}(\rho(t))\) decreases from 1 (the segregated and heterogeneous phase—the information diffuses from single nodes only to the local neighbourhood) to 0 (the integrated and homogeneous phase—the information has spread all over the network). The temporal derivative of the entropy, \(C(t) = -\frac{d}{dt} \log \mathcal{S}(\rho(t))\), represents the specific heat of the system, tightly linked with the system correlation lengths. In particular, a constant specific heat is a reflection of the scale-invariant nature of the network (Methods).

As shown in Fig. 1, for the specific case of Barabási–Albert (BA) networks and random trees (RTs), there is a characteristic loss of information as the time \(t\) increases. The larger the time, the lower the localized information on the different mesoscale network structures. From the analysis of the changes in the entropy evolution (Methods), together with its derivative, \(C\), the characteristic network resolution scales emerge\(^{25}\). Specifically, the peaks in the specific heat reveal the full network scale at significant diffusion times (scaling with the system size) and the short-range characteristic scales of the network (\(\tau\), tantamount to the lattice spacing \(a\) in well-known Euclidean spaces \(\mathbb{R}^d\)).

Real-space LRG

A crucial point is to extract the network ‘building blocks’, that is, to generate a metagraph at each time \(t\), to link the different network mesoscales. Note that, at time \(t=0\), \(\hat{\rho}\) is the diagonal matrix \(\rho_i(0) = \delta_{iN}\). Hence, \(\hat{\rho}(t)\) will be subject to the properties of the network Laplacian, ruling the current information flow between nodes, and will reflect the RG flow. So far, we need to consider a rule (in a similar way to the ‘majority rule’) to scrutinize the network substructures at all resolution scales (that is, \(\tau\)). For the sake of simplicity, we choose the following one: two
nodes reciprocally process information when they reach a value greater than or equal to the information contained on one of the two nodes\(^2\), thereby introducing \(\rho' = \min(\rho_i, \rho_j)\). Thus, depending on their particular \(\rho\), matrix element at time \(\tau\), it is possible to define the metagraph, \(\zeta = \Theta(\rho' - 1)\) where \(\Theta\) stands for the Heaviside step function. As expected, for \(\tau \to \infty\), \(\rho\) converges to \(\rho = 1/N\) and \(\zeta\) becomes a matrix with all 1’s.

For a given scale, the metagraph \(\zeta\) is thus the binarized counterpart of the canonical density operator, in analogy with the path-integral formulation of general diffusion processes\(^7\). Note that, after examining all continuous paths travelling along the network\(^8\) and starting from node \(i\) at time \(\tau = 0\), our particular choice selects the most probable paths from equation (1), giving information about the prominent information flow paths of the network in the interval \(0 < \tau < r\). In the language of the statistical mechanics, we are considering the analogy with the Wiener integral and building the RG diffusion flow of the network structure\(^9\). The last step is to recursively group the nodes of the network into subsequent supernodes, that is, the procedure in order to perform the process of node decimation.

In full analogy with the Kadonoff picture, it is possible to consider nodes—under the accurate selection of particular blocking scales of the network—within regions up to a critical mesoscale, which behave like a single supernode\(^12,38\). Analogously to the real-space RG, there is no unique way to generate new groups of supernodes or coarse grainings, but if the system is scale invariant, we expect it to be unaffected by RG transformations. In this perspective, using the specific heat, \(C\), we propose an RG rule over scales \(\tau \to \tau'\), where \(\tau'\) stands for the \(C\) peak at short times, realizing the small network scales. The renormalization procedure consists of the following steps (see also Fig. 2):

1. Build the network metagraph for \(\tau = \tau'\), that is, a set of heterogeneous disjoint blocks of \(n\) nodes extracted from \(\zeta\) (ref. 26).
2. Replace each block of connected nodes with a single supernode.
3. Consider supernodes as a single node incident to any edge of the original \(n\) nodes.
4. Realize the scaling.

Figure 3 shows the application of multiple steps \(L\) of the LRG over different networks. Note that Erdős–Rényi networks exhibit only a characteristic resolution scale (Supplementary Information Section 2). Kadonoff supernodes are, before this scale, only single nodes, making the network trivially invariant. For any possible grouping of nodes—at every scale, \(r\) —the mean connectivity of the network decreases after successive RG transformations. The network thus flows to a single-node state, reflecting the existence of a well-defined network scale (see further analysis and other test cases as in, for example, stochastic block models in Supplementary Information Section 2).

The LRG can also be applied to challenging networks of particular interest to real-life applications as well as small-world ones, revealing the possibility of making network reduction in this type of structure (even if they present intertwined scales, see Supplementary Information Section 2). Nonetheless, when performing RG analyses over bona fide scale-invariant networks, as in the BA model, both the mean connectivity and the degree distribution remain invariant after successive network reductions, conserving analogous properties to the original one (see Fig. 3 and Supplementary Information Section 4 for further analysis with \(m > 1\)). Figure 3a shows a graphical example of a three-step decimation procedure for a BA network with \(m = 1\) and \(N = 512\) nodes. Different colours at every transformation represent Kadonoff supernodes. Analogously, Fig. 3e shows the LRG procedure over Rasters, confirming the capability of our approach to perform network reduction on top of well-defined synthetic scale-invariant networks (see also Supplementary Information Section 3). Furthermore, Fig. 3f displays the scale-invariant nature of the Lateral for different downscaled BA replicas.

Finally, we apply the LRG to different scale-free real networks, that is, following bona fide finite-size scaling hypotheses\(^3\), and significant cases previously analysed in other RG approaches\(^3\), producing down-scaled network replicas. Figure 4 shows the particular case of Arabidopsis Thaliana\(^2\) and Drosophila Melanogaster\(^39\) metabolic networks (confirming the scale-free inherent nature of these networks), the Human HI-II-14 interactome\(^10\) and the Internet Autonomous system\(^11\) (see Supplementary Information Section 5 for a significant number of examples).

**LRG**

Thus far, as in the Kadonoff hypothesis, we do not have a clear justification for our assumptions. In this section, we introduce a rigorous formulation of the LRG, which can be appropriately seen as the analogue of the field theory \(k\)-space RG following that of Wilson\(^40\) in statistical physics. From this formulation, we get a Fourier-space version of Kadonoff’s supernode scheme at each LRG step. We also give a real-space interpretation of this procedure.

Without loss of generality, let us consider the case in which we want to renormalize the information diffusion on the graph up to a time \(\tau^*\) so as to keep only diffusion modes on scales larger than \(\tau\) (for example, where \(C\) shows a maximum). Let us adopt the bra–ket formalism in which \(|i\rangle\langle j|\) indicates the projection of the Laplacian eigenvector \(|\lambda|\) on the \(i\)th node of the graph. In this sense we can identify \(|j|\) with the normalized \(N\)-dimensional column vector that has all components as 0 with the exception of the \(i\)th component, which is 1. In the bra–ket notation, the Laplacian operator is \(\sum|\lambda|\langle\lambda|\lambda|\rangle\). We then identify the \(n < N\) eigenvalues \(\lambda \approx \lambda^* = 1/N\) and the relative eigenvectors \(|\lambda|\). A LRG step consists of integrating out these diffusion eigenmodes from the Laplacian and appropriately rescaling the graph, namely:

1. We reduce the Laplacian operator to the contribution of the \(N - n\) slow eigenvectors with \(\lambda \approx \lambda^*\).
2. We then rescale the time \(\tau \to \tau'\), so that \(\tau'\) becomes the unitary interval in the rescaled time variable \(\tau' = \tau/\tau^*\), and consequently redefine the coarse-grained Laplacian as \(\mathcal{L}'^* = \tau^* \mathcal{L}'\). Apart from the temporal rescaling, this \(k\)-space LRG scheme can be represented in real-space through the formation of \(N - n\) supernodes from the \(N\) original graph nodes using the operator \(\mathcal{P}^*\); by ordering the values of \(|\rho_{ij}(\tau^*)| = |\langle i| \mathcal{P}^* |j|\rangle|\) in descending order, we can follow this ordered list to aggregate the nodes, stopping when \(N - n\) clusters/supernodes are obtained. Note that, in the original basis of \(N\) nodes, these supernodes are represented by \(N - n\) orthogonal vectors \(|\alpha|\) with \(\alpha = 1, \ldots, N - n\), which can be used as a reduced \((N - n)\)-dimensional basis to represent both the coarse-grained Laplacian operator \(\mathcal{L}'\) and the corresponding adjacency matrix \(A': A'_{\alpha\beta} = -\rho_{\alpha\beta} = -|\langle \alpha| \mathcal{L}' |\beta|\rangle|\), for \(\alpha \neq \beta\). Moreover, we set \(A'_{\alpha\alpha} = 0\) and \(L_{\alpha\alpha} = \sum_\beta A'_{\alpha\beta}\).
It is crucial to note that, as defined above, this formulation of the LRG malization step of the graph, reducing the dimension from $N$ to $N-m$. Section 4 for further examples with at different RG steps with $\kappa$, for a BA network (solid lines), with a characteristic exponent $\gamma$ different colour for every scale.

Conclusions

The RG represents a significant development in contemporary statistical mechanics. Its application to diverse dynamical processes operating on top of regular spatial structures (lattices) allows the introduction of the idea of universality and the classification of models (otherwise presumed faraway) within a small number of universality classes. Examples run from ferromagnetic systems, to percolation to polymers. Recently, groundbreaking applications have addressed the problem in complex biological systems, illuminating collective behaviour of neurons in mouse hippocampus or dynamical couplings in natural swarms.

There is no apparent equivalence to analysing RG processes in complex spatial structures, even if some pioneering approaches have recently proposed sound procedures that can state equivalent general RG schemes to those of statistical physics. The most promising approaches draw on hidden metric assumptions, spatially mapping nodes in some abstract topological space, which must be considered as an ‘a priori’ hypothesis. Despite this, they show fundamental problems in maintaining the intrinsic network properties—for example, connectivity—of reduced replicas when performing decimation. Moreover, setting the equivalent to conventional RG flow without any spatial projection of the nodes or grouping premises, but induced by diffusion distances, remains an unsolved fundamental problem.

Here we develop an RG scheme based on information diffusion distances, taking advantage of the fact that the Laplacian operator is a spatial projection of the nodes or grouping premises, but induced by diffusion distances, remains an unsolved fundamental problem.
the Kadanoff blocking scheme, that is, the blocks need to reflect the intrinsic heterogeneous architecture of the network. This conundrum automatically leads to many possibilities in grouping nodes, making the problem seem unsolvable.

The study of the Laplacian spectrum (which defines the conjugate Fourier space) allows us to compute the network modes, playing the exact role of $a$ and $A$ (the microscopic ultraviolet cut-off) in RG schemes. We point out that to select critical scales of the network, all eigenvalues (fluctuations) can be of utmost relevance to give us information about the intertwined network scales, relating the short-distance cutoff and the macroscopic scale. In particular, our framework conserves the main network properties—for example, the average degree—of the downscaled networks (only if they are truly scale invariant), thus confirming the existence of repulsive, non-trivial, fixed points in the RG flow. It also allows us to extract mesoscopic information concerning the network communities even if they are blatantly scale dependent. Our RG scheme solves a crucial open problem: the limited iterability in small-world networks due to short path lengths, limited only by network size.

Altogether, we propose here a new RG approach following that of Wilson—therefore working in the momentum space—based on the Laplacian properties of the network: the LRG, which is the natural extension to heterogeneous networks of the usual RG approach in statistical physics and statistical field theory. We demonstrate that only scale-invariant networks will exhibit constant specific-heat values at all resolution scales reflecting some sort of translational invariance, even if it is possible to define scale-free structures that can some how be renormalized. BA networks that present ultra-small-world properties are a prime example of this (they are scale invariant only for $n = 1$, see Supplementary Information Section 4), and are therefore the counterpart of the trees to the Watts–Strogatz process in lattices.

Our LRG scheme opens a route to extend RG flow study further, developing a common mathematical framework classifying complex networks in universality classes. Finally, subsequent analyses can also help in shedding light on the interplay between structure and dynamics through the analysis of specific RG flows and emergent fixed points for multiple dynamical models.

**Online content**

Any methods, additional references, Nature Portfolio reporting summaries, source data, extended data, supplementary information, acknowledgements, peer review information; details of author contributions and competing interests; and statements of data and code availability are available at https://doi.org/10.1038/s41567-022-01866-8.

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Methods

Statistical physics of information network diffusion

Let us consider the adjacency matrix of a simple binary graph, $A$, and define $L = D - A$ as the ‘fluid Laplacian matrix’\(^{18}\), where $D_i = \delta_i \delta_i$ and $\delta_i$ is the connectivity of the node $i$. In terms of the network propagator, $\hat{K} = e^{-\tau L}$, it is possible to define the ensemble of accessible information diffusion states\(^{13,14,36}\), namely,

$$\hat{\rho}(\tau) = \frac{e^{-\tau L}}{Z}. \quad (3)$$

where $\hat{\rho}(\tau)$ is tantamount to the canonical density operator in statistical physics (or to the functional over fields configurations)\(^{13,14,36}\), and $Z = \sum_{\tau} e^{-\tau L}$, with $\lambda_i$ being the set of system eigenvalues. Since, for a simple graph, $L$ is a Hermitian matrix, $\hat{L}$ plays the role of the Hamiltonian operator and $\tau$ the role of the inverse temperature. It is possible to therefore define the network entropy\(^25\) through the relation

$$S(\hat{\rho}(\tau)) = -\text{Tr} [\hat{\rho}(\tau) \log \hat{\rho}(\tau)] = \text{Tr} [\frac{e^{-\tau L}}{Z} (\tau L + \log Z)] = \tau \langle \lambda \rangle_\tau + \log Z \quad (4)$$

with $(\hat{\Omega}_\tau = \text{Tr}[\hat{\rho}\hat{\Omega}])$. Immediately, it is possible to define the specific heat of the network as

$$C(\tau) = -\frac{dS}{d\log \tau} = -\tau^2 \frac{d\langle \lambda \rangle_\tau}{d\tau} \quad (5)$$

Informational phase transitions

The specific heat of the network of equation (5) is a detector of transition points corresponding to the intrinsic characteristic diffusion scales of the network. In particular, the condition $\frac{d\langle \lambda \rangle_\tau}{d\tau} \bigg|_{\tau = \tau_c} = 0$ defines $\tau_c$, and reveals the existence of pronounced peaks revealing a strong deceleration of the information diffusion. Moreover, employing the thermal fluctuation-dissipation theorem\(^23\), the specific heat links to entropy fluctuations\(^23\) making $C$ proportional to $\sigma^2_t = \langle S^2 \rangle - \langle S \rangle^2$, which, over many independent realizations, scales as $1/N$, where $N$ is the number of nodes of the network (as a direct application of the central limit theorem\(^{30,49}\)).

Scale-invariant networks

Let us now define informationally scale-invariant networks in agreement with our definition of the LRG. A network has scale-invariant properties in a resolution region if the entropic susceptibility/specific heat $C$ takes a constant value $C_i > 0$ in the corresponding diffusion time interval. This property describes a situation in which the informational entropy increases by the same amount in two equal logarithmic time scales, which means a scale-invariant transmission of the information at every network resolution scale. It is matter of simple algebra to see, from equation (5), that this means

$$\frac{d\langle \lambda \rangle_\tau}{d\tau} = -\frac{C_i}{\tau^2}. \quad (6)$$

Knowing that, for $\tau \to \infty$, $\langle \lambda \rangle \to 0$, by integration we find

$$\langle \lambda \rangle_\tau = \frac{C_i}{\tau} \sum_{i=1}^N \lambda_i e^{-\tau \lambda_i} / \sum_{i=1}^N e^{-\tau \lambda_i}. \quad (7)$$

In the continuum approximation of the Laplacian spectrum, equation (6) implies a power-law eigenvalue density function $P(\lambda) = \lambda^y$ for small $\lambda$, that is, large diffusion times, with the exponent $y$ satisfying the following relation:

$$C_i = \frac{\Gamma(y+2)}{\Gamma(y+1)} = y+1, \quad (7)$$

where $\Gamma(z)$ is the Euler gamma function.

Data availability

All the data supporting the results presented in this paper are available from the corresponding author upon reasonable request.

Code availability

All the codes supporting the results presented in this paper are available from the corresponding author upon reasonable request.

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Author contributions

All authors designed the research. P.V. performed the computational simulations and data analysis. A.G. developed the mathematical framework. All authors wrote the paper.

Competing interests

The authors declare no competing interests.

Additional information

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