Network evolution towards optimal dynamical performance

Studienstiftung des deutschen Volkes

bcgs

Bonn-Cologne Graduate School of Physics and Astronomy

STEFFEN KARALUS AND MARKUS PORTO

Institut für Theoretische Physik, Universität zu Köln, Germany

Summary

The functionality of many empirical networks is provided by dynamical processes based on the network structure. Evolving networks commonly change their structure due to the resulting dynamical behavior. A deeper understanding of the interplay between the network topology and the dynamical behavior should therefore provide valuable insight into the structure-function relationship of networked systems. We present a generic approach to investigate this relationship which is applicable to a wide class of dynamics, namely to evolve networks using a performance measure based on the whole spectrum of the dynamics' time evolution operator. As basic example we consider the graph Laplacian, the relevant operator for many fundamental processes such as diffusion or synchronization, and show that our algorithm successfully evolves networks into states with a given desired behavior. Interestingly, the resulting networks show an overall trend towards heterogeneous structures, whereas the dynamical heterogeneity is rather small.

Introduction

Goal: Optimize the network structure for a desired dynamical behavior of a dynamical process taking place on the network.

Dynamical processes on networks

- Network of N vertices and M edges
- Dynamical state of vertices

$$\mathbf{p}(t) = (p_1(t), \dots, p_N(t))^{\mathrm{T}}$$

- Linear dynamics

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p}(t) = \mathscr{O}\,\mathbf{p}(t)$$

Time evolution operator $\mathscr{O}$

- Incorporates interaction pattern (network topology)
- Eigenvalues λ_ν determine the dynamical behavior

Evolutionary Optimization

Spectral representation by **integrated density of states (DOS)** function

$$I(\lambda) = \frac{1}{N}\sum_{\nu=1}^{N}\Theta(\lambda - \lambda_\nu)$$

Desired dynamical behavior defined by **target integrated DOS**

$$I^{\text{target}}(\lambda)$$

Quantify dynamical performance of a network by **distance measure** to target integrated DOS

$$d(I, I^{\text{target}})$$

Evolution of network structure by successive steps of

- **Mutation:** Create candidate network by random topology changes
- **Selection:** Acceptance of candidate by criterion based on distance measure

Diffusion Processes

Time evolution operator: **Graph Laplacian**

$$L_{ij} = \delta_{ij}k_i - A_{ij} = \begin{cases} k_i & \text{if } i = j\,, \\ -1 & \text{if vertex } i \text{ linked to vertex } j\,, \\ 0 & \text{otherwise}\,. \end{cases}$$

Diffusion equation

$$\frac{\mathrm{d}}{\mathrm{d}t}\mathbf{p}(t) = -C\,\mathbf{L}\,\mathbf{p}(t)$$

Characterized by **probability of returning to origin**

$$P_0(t) \propto t^{-d_s/2}$$

Power law scaling of integrated DOS

$$I(\lambda) \propto \lambda^{d_s/2}$$

Spectral dimension of normal diffusion

$$d_s^{(n)} = 2$$

Evolution goal: **Sub-diffusion** with given

$$d_s^{(1)} = 1.4\,, \qquad d_s^{(2)} = 1.1$$

Rescaled eigenvalues of graph Laplacian

$$\tilde{\lambda}_\nu = \frac{\lambda_\nu}{\max_{\nu'}\{\lambda_{\nu'}\}}$$

Logarithmically integrated DOS

$$\tilde{I}(\log\tilde{\lambda}) = \log\left(\frac{1}{N}\sum_{\nu=1}^{N}\Theta(\log\tilde{\lambda} - \log\tilde{\lambda}_\nu)\right)$$

Distance measure

$$d(\tilde{I}, \tilde{I}^{\text{target}}) = \int_{\log\tilde{\lambda}_{\min}}^{0}\left|\tilde{I}(\log\tilde{\lambda}) - \tilde{I}^{\text{target}}(\log\tilde{\lambda})\right|^2 \mathrm{d}\log\tilde{\lambda}$$

Evolution step:

- **Mutation:** Move one edge to other pair of vertices
- **Selection:** Accept if distance measure decreases

→ The system performs an **adaptive walk** in space of networks with fixed numbers of vertices and edges.

Acknowledgements

We gratefully acknowledge helpful discussions with Sebastian Weber in early stages of this work and funding by the *Studienstiftung des deutschen Volkes* and the *Bonn-Cologne Graduate School of Physics and Astronomy* (SK) and the *Deutsche Forschungsgemeinschaft* via the Heisenberg program (PO 1025/6) (MP).

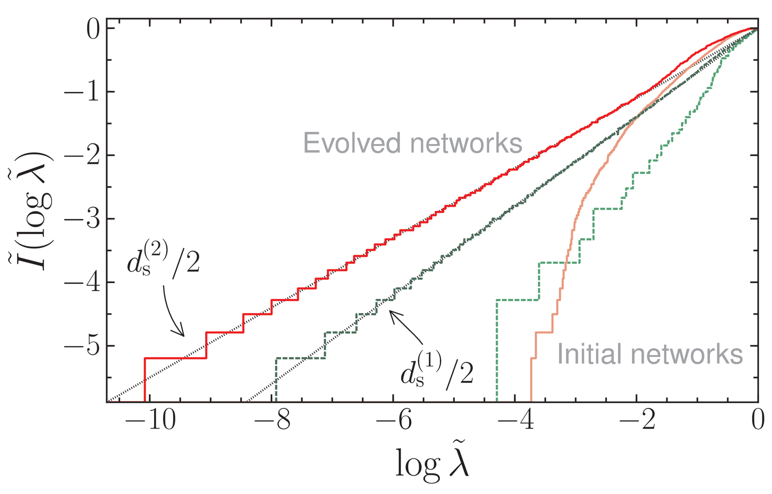
Results

Independent evolution runs starting from

- 2d square lattices with periodic boundary conditions → **Green curves**
- Connected random graphs with fixed N and M $G(N,M)$ → **Red curves**

Evolutions run for $n = 10^6$ steps

Logarithmically integrated density of states



Initial networks (light colors)

Final networks (dark colors)

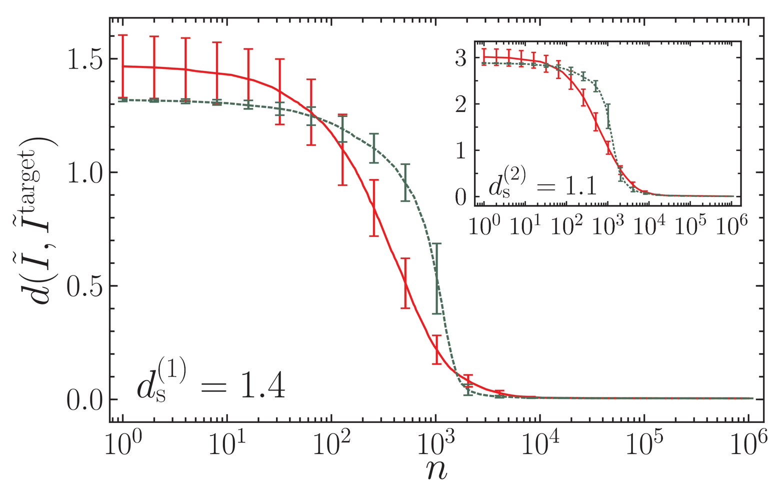
Target DOS (black dotted)

Integrated DOS converges towards respective target

Evolution of distance measure

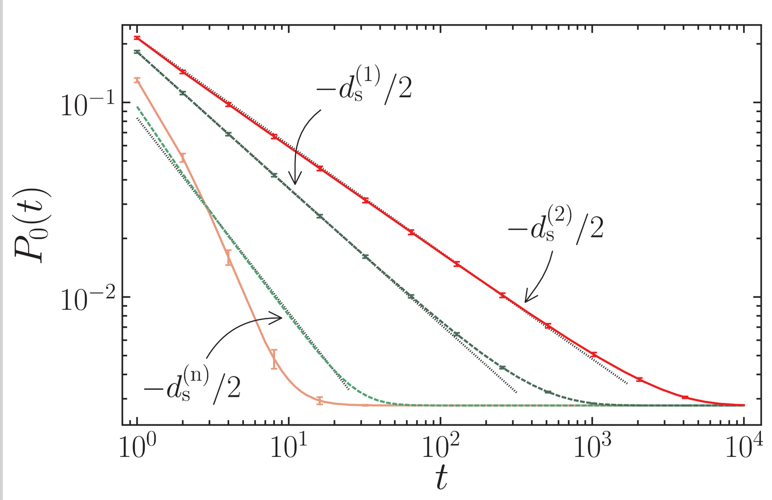
Two initial states (red/green)

Two targets (main/inset)



- Convergence after ~10^4 steps in all four cases
- No distinction between different initial states

Average return probability



Lattice → $d_s^{(1)}$ (green)

$G(N,M)$ → $d_s^{(2)}$ (red)

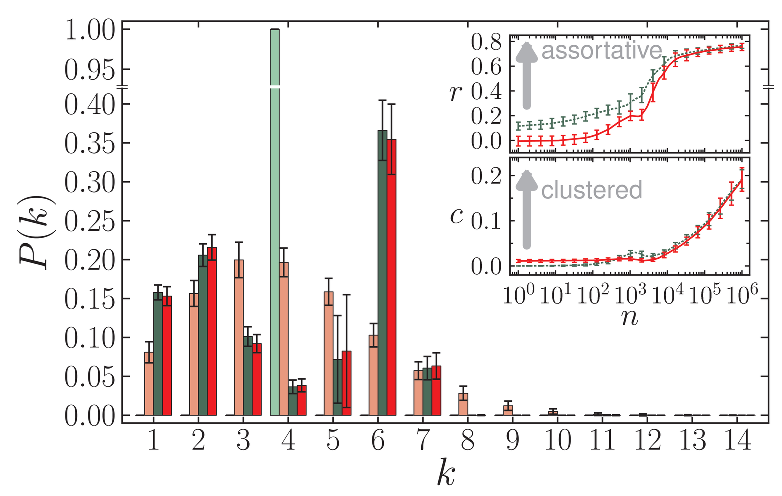
Expected scaling (black dotted)

- Scaling nicely fits expectation
- Small dynamical heterogeneity (error bars)

Degree distribution, assortativity and clustering coefficients of evolved networks

Evolutions:

Lattice / $G(N,M)$ → $d_s^{(1)}$



- Degree distribution becomes broader
- Networks become assortative and clustered → High structural heterogeneity