Optimizing the Gillespie algorithms for simulating spreading phenomena in higher-order networks

Hugo P. Maia[1], Wesley Cota[1] and Silvio C. Ferreira[1,2]

[1] *Departamento de Física, Universidade Federal de Viçosa - Viçosa, MG, Brazil*
[2] *Instituto Nacional de Ciência e Tecnologia de Sistemas Complexos - INCT-SC*

hugo.maia@ufv.br, wesley.cota@ufv.br, silviojr@ufv.br

Introduction

Higher-order networks are a generalization on traditional pairwise networks. Instead of edges connecting only pairs of nodes, systems may now include hyperedges that represents group interactions between any number of nodes. Due to this increased complexity, simulation of contagion dynamics often culminates in either inefficient or inaccurate algorithms.

Higher-Order Contagion

A hypergraph $\mathscr{H} = \{\mathscr{N}, \mathscr{E}\}$ is a type of higher-order network defined by a set of nodes $\mathscr{N} = \{i_1, i_2, i_3, ..., i_N\}$ and a set of hyperedges $\mathscr{E} = \{h_1, h_2, h_3, ..., h_H\}$.

A node's generalized degree or m-degree $k_i^{(m)}$ refers to the number of i's m-hyperedges. A hyperdegree is defined as the set of generalized degrees, $\mathbf{k_i} = \{k_i^{(1)}, k_i^{(2)}, k_i^{(3)}, ...\}$, each node having $K_i = \sum_m k_i^{(m)}$ interactions in total.

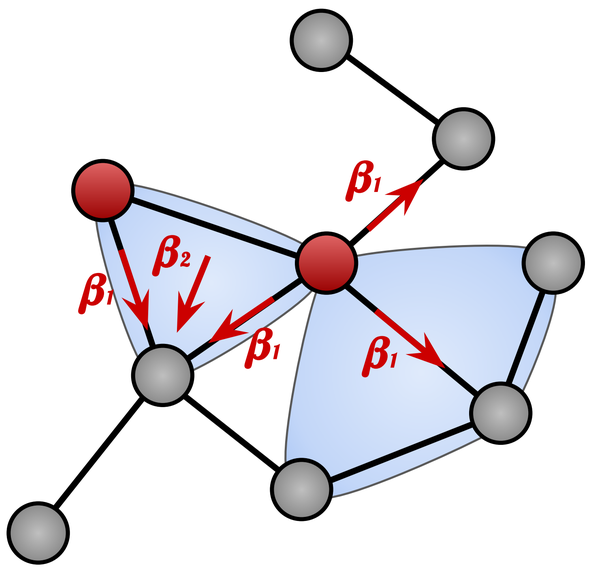


Fig. 1: Example of the Hyper-SIS contagion model on a higher-order network. Susceptible nodes ($\sigma_i = 0$) are indicated in gray and infected ones ($\sigma_i = 1$) in red.

The Hyper-SIS model with critical mass threshold assumes that only $\theta_m \in [1, m]$ from all $m+1$ agents are necessary to activate an m-order hyperedge and transmit the infection at a rate $\beta^{(m)}$. A hyperedge h is active if $\sum_{i \in h} \sigma_i \geq \theta_m$. Events are represented by the equations

$$\mathrm{I} \xrightarrow{\alpha} \mathrm{S}, \quad \text{and} \quad \theta_m \mathrm{I} + \mathrm{S} \xrightarrow{\beta^{(m)}} (\theta_m + 1)\mathrm{I}.$$

We employ a vector notation for higher order parameters, such as the spreading rates $\beta = \{\beta^{(1)}, \beta^{(2)}, \beta^{(3)}, ...\}$ and hyperdegrees $\mathbf{k} = \{k^{(1)}, k^{(2)}, k^{(3)}, ...\}$.

Generating Higher-Order Networks

The bipartite configuration model is used to create synthetic higher-order networks with predefined number of interactions and order distribution.

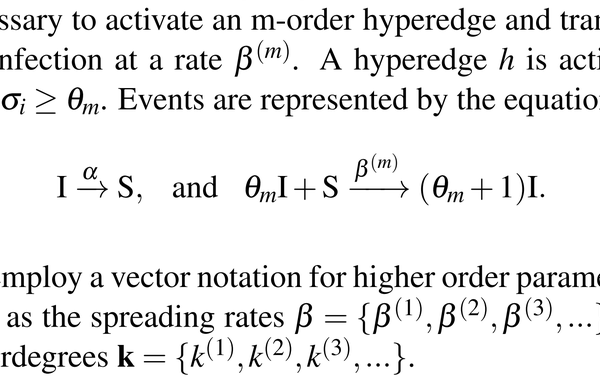
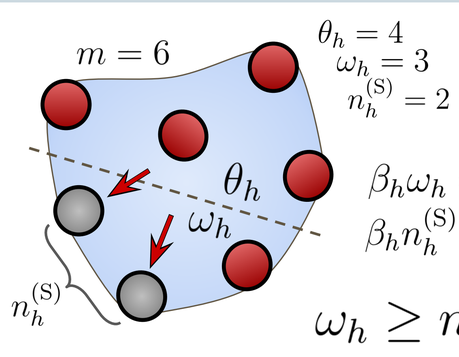


Fig. 2: Steps employed to construct higher-order networks via the bipartite configuration model.

1. Create sets of nodes with distributions P_k^A and P_k^B. The total sum of degrees in A must be equal to that of B, i.e $S_k^A = \sum_{i \in A}^{N_A} k_i = S_k^B = \sum_{i \in B}^{N_B} k_i$.
2. Randomly connect nodes from both partitions. Nodes from partition A and B must connect to each other at most only once, and no hyperedges of the same order can contain the same sets of nodes.
3. The resulting bipartite graph is reinterpreted as a higher-order network with the predefined interaction and order distributions.

Results

Hyperedge-Based Optimized Gillespie Algorithm



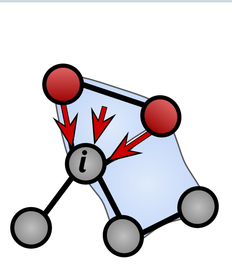
$$\beta_h \omega_h = 3\beta^{(6)}$$
$$\beta_h n_h^{(S)} = 2\beta^{(6)}$$
$$\omega_h \geq n_h^{(S)}$$

For the HB-OGA, a list $\Lambda^{(\mathrm{act})}$ contains all active hyperedges ($\sigma_h^{(act)} = 1$). We overestimate the number of possible processes by assuming that an active hyperedge spreads the infection to $\omega_m = m + 1 - \theta_m$ of its nodes at a rate $\beta^{(m)}$, resulting in a total infection rate

$$B = \sum_{h=1}^{H} \beta_h \omega_h \sigma_h^{(act)} = \sum_m \beta^{(m)} \omega_m N_{\mathrm{act}}^{(m)}.$$

For infection events, a hyperedge is selected from the list $\Lambda^{(\mathrm{act})}$ and accepted proportionally to $\beta_h \omega_h$, then with probability $n_h^{(S)}/\omega_h$ one of its susceptible nodes is infected, otherwise resulting in a phantom process. Whatever the outcome, time is incremented by $\tau = -\ln u/(\alpha N_{\mathrm{inf}} + B)$.

Node-Based Optimized Gillespie Algorithm



$$\vec{k_i} = \{4, 1, 1\}$$
$$\vec{k_i} \cdot \vec{\beta} = 4\beta^{(1)} + \beta^{(2)} + \beta^{(3)}$$
$$\vec{n_i} = \{2, 1, 0\}$$
$$\vec{n_i} \cdot \vec{\beta} = 2\beta^{(1)} + \beta^{(2)}$$
$$k_i^{(m)} \geq n_i^{(m)}$$

For the NB-OGA, a list $\Lambda^{(\mathrm{qui})}$ contains all nodes that belong to active hyperedges ($\sigma_i^{(\mathrm{qui})} = 1$). It is assumed that quiescent nodes acquire the infection at a rate $\beta^{(m)}$ from every $k_i^{(m)}$ of its m-order hyperedges, resulting in an overestimated total infection rate

$$B = \sum_{i=1}^{N} \left(\sum_m \beta^{(m)} k_i^{(m)} \right) \sigma_i^{(\mathrm{qui})} = \sum_m \beta^{(m)} N_e^{(m)}.$$

For infection events, a quiescent node is selected from the list $\Lambda^{(\mathrm{qui})}$ and accepted proportionally to $\vec{\beta} \cdot \tilde{\mathbf{k}}_\mathbf{i}$, then the node i is infected with probability $\vec{\beta} \cdot \tilde{\mathbf{n}}_i / \vec{\beta} \cdot \tilde{\mathbf{k}}_i$, otherwise resulting in a phantom process. Time is incremented by $\tau = -\ln u/(\alpha N_{\mathrm{inf}} + B)$.

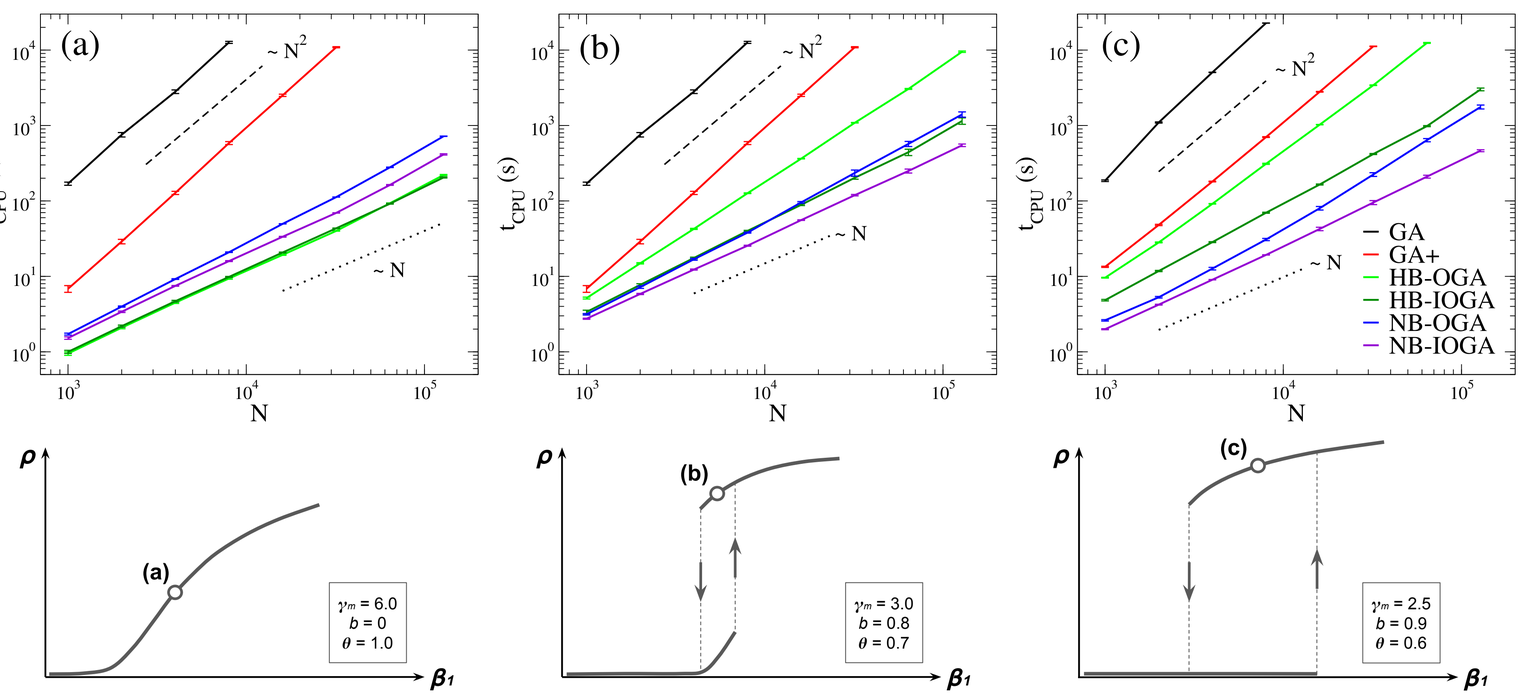


Fig. 3: Algorithm comparison for the simulation of the hyper-SIS model on higher-order networks with power-law interaction $P_K \sim K^{-\gamma_k}$ and order $P_m \sim m^{-\gamma_m}$ distributions. Figures above are CPU time with relation to network size, and figures below are schemes for the points tested in the simulation. Numerical data is shown in a table below.

	GA	GA+		HB-OGA (IOGA)			NB-OGA (IOGA)		
N	8000	8000	32000	8000	32000	128000	8000	32000	128000
Homogeneous$^{(a)}$	308	3.83	54.0	0.16	0.77	3.51	0.32	1.38	6.05
Homogeneous$^{(b)}$	–	23.9	–	0.65	3.00	14.0	0.54	2.36	10.3
Simplicial Complex$^{(a)}$	–	164	–	0.61	3.01	12.5	0.58	2.58	13.7
Simplicial Complex$^{(b)}$	–	49.3	–	0.33	1.47	6.28	0.32	1.49	7.79
PL, $\gamma_m = 6.0^{(a)}$	210	9.73	181	0.15 (0.16)	0.66 (0.72)	3.68 (3.41)	0.34 (0.26)	1.87 (1.15)	12.0 (6.89)
PL, $\gamma_m = 3.0^{(b)}$	545	13.1	223	2.11 (0.66)	18.1 (3.38)	158 (19.1)	0.63 (0.42)	3.91 (1.98)	23.3 (9.12)
PL, $\gamma_m = 2.5^{(c)}$	379	11.7	186	5.17 (1.16)	56.4 (6.98)	– (50.1)	0.51 (0.32)	3.73 (1.58)	29.3 (7.72)
hyperblob$^{(a)}$	1142	10.3	162	8.72 (7.50)	138 (115)	– (–)	0.86	15.0	247
hyperblob$^{(b)}$	–	31.8	652	1073 (34.0)	– (569)	– (–)	0.86	15.0	247

Conclusions

- Higher-order systems are the next step in network sciences, filled with new and unique emergent phenomena.
- The algorithms proposed here optimizes simulation of higher-order contagion processes by orders of magnitude and for several types of networks with different levels of heterogeneity.
- Optimizations can be adapted and employed for a multitude of contagion models with different rules and compartments.

Financial Support: CNPq, FAPEMIG and CAPES

References

[1] F. Battiston, E. Amico, A. Barrat, G. Bianconi, G. Ferraz de Arruda, B. Franceschiello, I. Iacopini, S. Kéfi, V. Latora, Y. Moreno, et al., "The physics of higher-order interactions in complex systems," *Nature Physics*, vol. 17, no. 10, pp. 1093–1098, 2021.

[2] W. Cota and S. C. Ferreira, "Optimized gillespie algorithms for the simulation of markovian epidemic processes on large and heterogeneous networks," *Computer Physics Communications*, vol. 219, pp. 303–312, 2017.

[3] G. Cencetti, D. A. Contreras, M. Mancastroppa, and A. Barrat, "Distinguishing simple and complex contagion processes on networks," *Phys. Rev. Lett.*, vol. 130, p. 247401, 2023.