Hypergraphs beyond directedness: heterogeneity and spectral centralities

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COMPLEX NETWORKS

Three colliding views on (hyper)edge directionality

Hypergraphs have been on the rise for the last decade. However, little to no attention has been paid to non-undirected interactions.

In graphs, the translation between sets, matrix components and topological structures is clear. In hypergraphs, until recently [1] the only description of non-undirected interactions was set-theoretic [2].

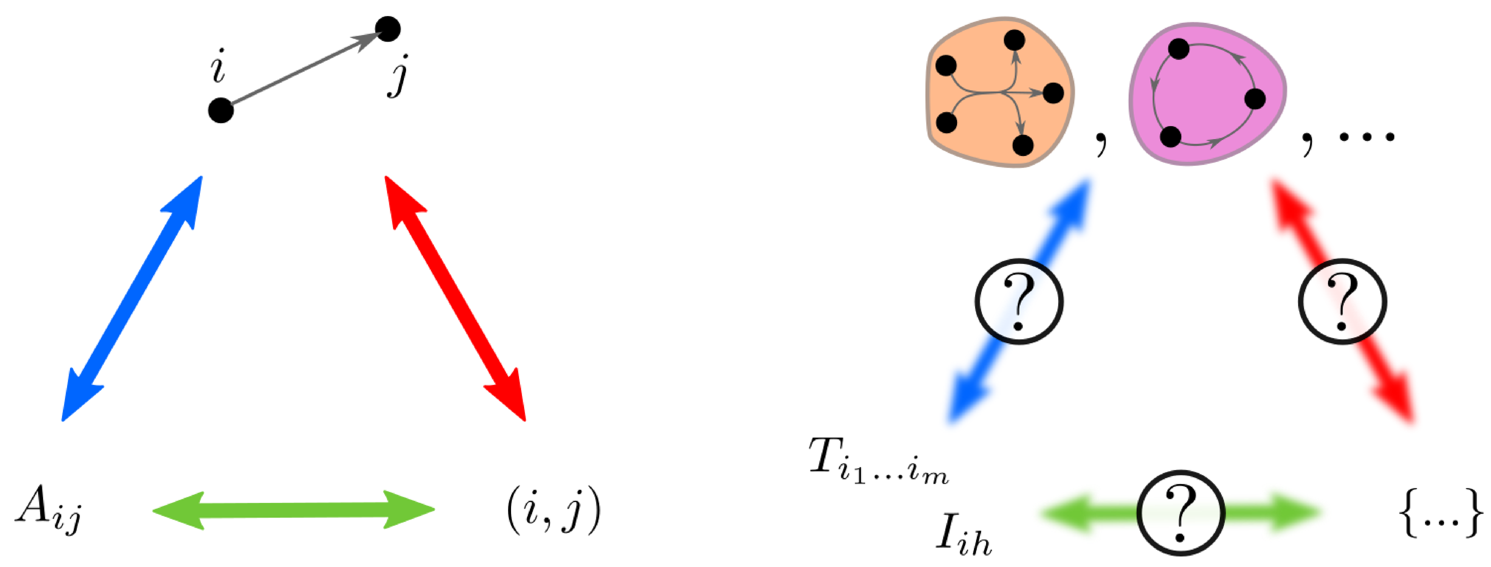

Figure 1. Topological, algebraic and set-theoretic perspective of a directed edge (left) and hyperedge (right).

Set theory point of view (old)

Directed hyperedges [2] are tuples $E_k = (T(E_k), H(E_k))$ where $T(E_k)$ is the tail set ("input" nodes) and $H(E_k)$ is the head set ("output" nodes) of the interaction.

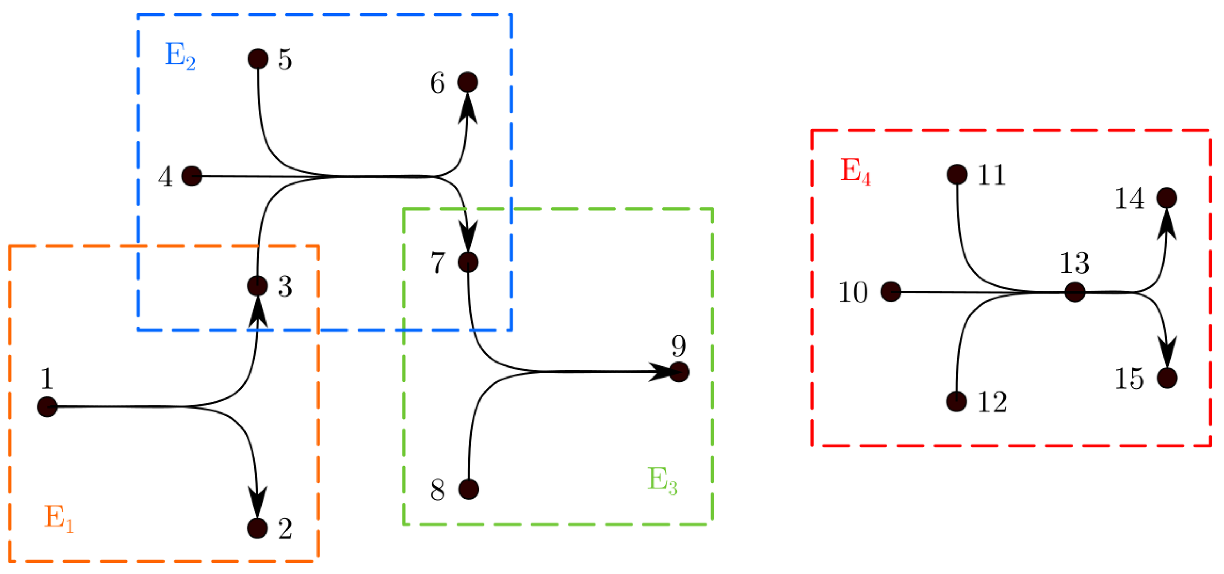

Figure 2. Example of directed hyperedges.

This perspective is rather limiting: it can't even describe something as simple as E_4 in Figure 2.

Algebraic point of view (new)

Hyperedges correspond to components of the adjacency hypermatrices $A_{ij}, T^{(3)}_{ijk}, T^{(4)}_{ijkl}, \ldots$

A hypergraph specified from its adjacency hypermatrices is "heterogeneous" [1]. Underlying symmetries accommodate other types:

- **Undirected:** for any permutation σ
$$T^{(k)}_{i_1\ldots i_k} = T^{(k)}_{\sigma(i_1\ldots i_k)}. \quad (1)$$
- **Cyclical:** for any odd or even permutation σ
$$T^{(k)}_{i_1\ldots i_k} = T^{(k)}_{\sigma(i_1\ldots i_k)}. \quad (2)$$
- **Directed:** for any permutations $\sigma^{\text{in}}, \sigma^{\text{out}}$
$$T^{(k)}_{i_1\ldots i_s i_{s+1}\ldots i_k} = T^{(k)}_{\sigma^{\text{in}}(i_1\ldots i_s)\sigma^{\text{out}}(i_{s+1}\ldots i_k)}. \quad (3)$$
- etc.

Application to spectral centralities

Benson defined the eigenvector centrality of undirected hypergraphs [3], based on the spectral theory of hypermatrices and satisfying existence theorems. The $\mathcal{H}$-eigenvector centrality is defined as

$$\lambda c_{i_1}^{k-1} = \sum_{i_2,\ldots,i_k=1}^{N} T^{(k)}_{i_1 i_2\ldots i_k} c_{i_2}\ldots c_{i_k}, \quad c_i > 0\ \forall i. \quad (4)$$

In [1], we extended this centrality measure to three types of heterogeneous hypergraphs cyclical, directed and k-step, after suitably defining the transposition of a hypermatrix.

Example: chemical interactions

We constructed several hypergraphs. Among them, directed ones of astrochemical reactions, using data from [4], and computed their spectral centralities.

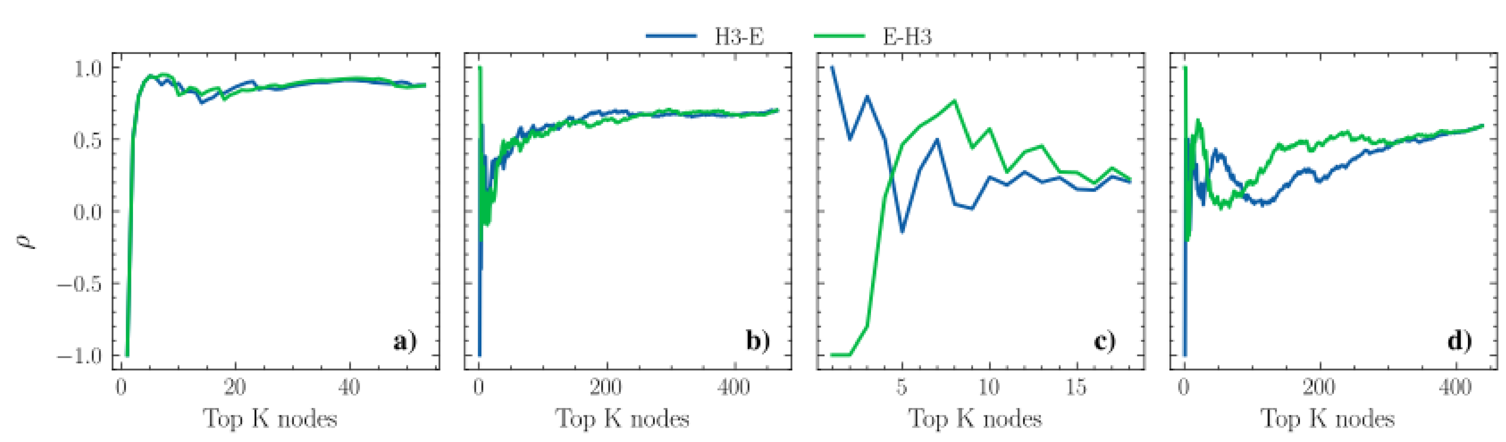

Figure 3. Spearman' ρ correlation between eigenvector centrality (EC) and $\mathcal{H}$-eigenvector centrality (HEC).

References

[1] G. Contreras-Aso et al. "Beyond directed hypergraphs: heterogeneous hypergraphs and spectral centralities" *Journal of Complex Networks, Volume 12, Issue 4, 2024.*

[2] G. Gallo et al. "Directed hypergraphs and applications" *Discrete Applied Mathematics, Volume 42, 1993.*

[3] A. R. Benson. "Three Hypergraph Eigenvector Centralities", *SIAM Journal on Mathematics of Data Science, Volume 1, Issue 2, 2019.*

[4] P. P. Plehiers et al. "Automated reaction database and reaction network analysis: extraction of reaction templates using cheminformatics". *Journal of Cheminformatics 10.1, 2018.*

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