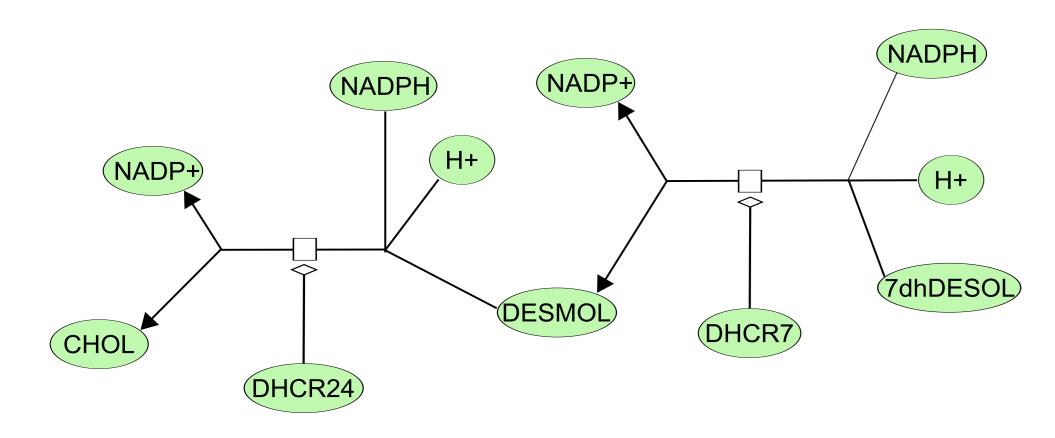


Hypergraphs: Algorithms, Implementations, and Applications Brendan Avent¹, Anna Ritz¹, and T. M. Murali ^{1,2}

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Motivation

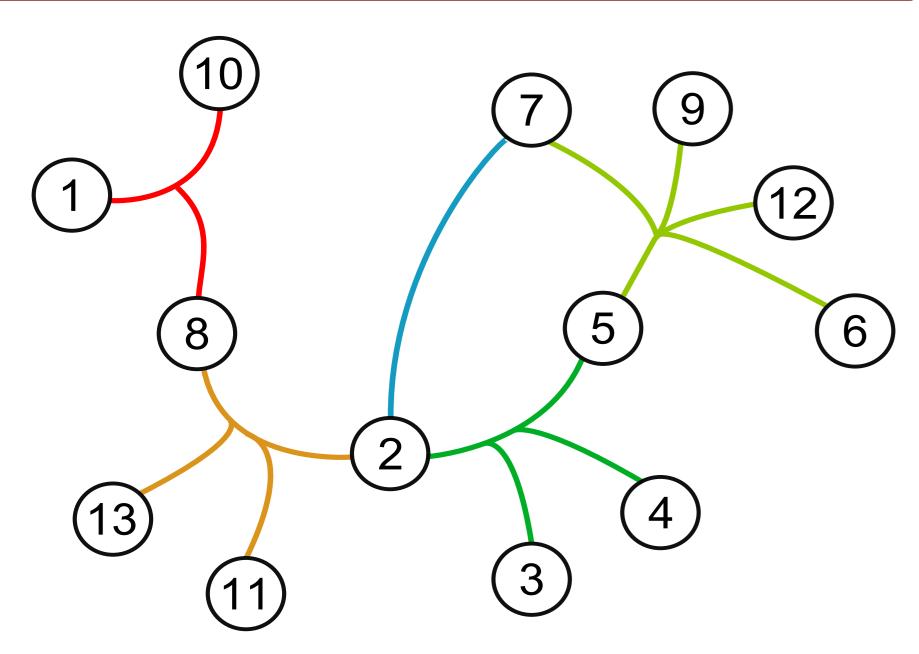
- Networks are ubiquitous in modern science, engineering, and the humanities
- ► Networks modeled with graphs can only represent pairwise interactions, not higher-order relationships



- Many software libraries for graphs exist: NetworkX, Boost, JUNG, etc.
- ► Challenge: no libraries for hypergraphs exist that have both data structures and algorithms. This leaves a lot of work to do!

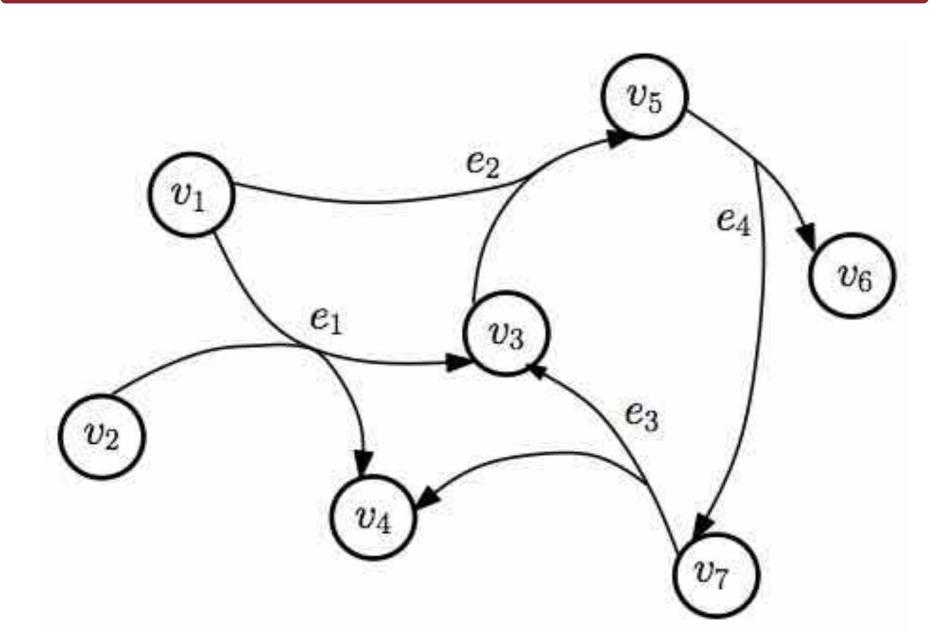
What Are Hypergraphs?

Undirected Hypergraphs



Undirected hyperedges connect groups of nodes.

Directed Hypergraphs



Directed hyperedges connect "tail" groups of nodes to "head" groups of nodes.

halp: Hypergraph Algorithms Package

Features

Open Source: Thoroughly tested Python package publicly-available on GitHub [1]

Data Structures: Directed and undirected hypergraph data structures to easily model complex networks

Usable Algorithms: Implementations of important and canonical hypergraph algorithms

Utilities: Quick extraction of hypergraph properties and statistics + conversion to other formats/structures

Algorithms

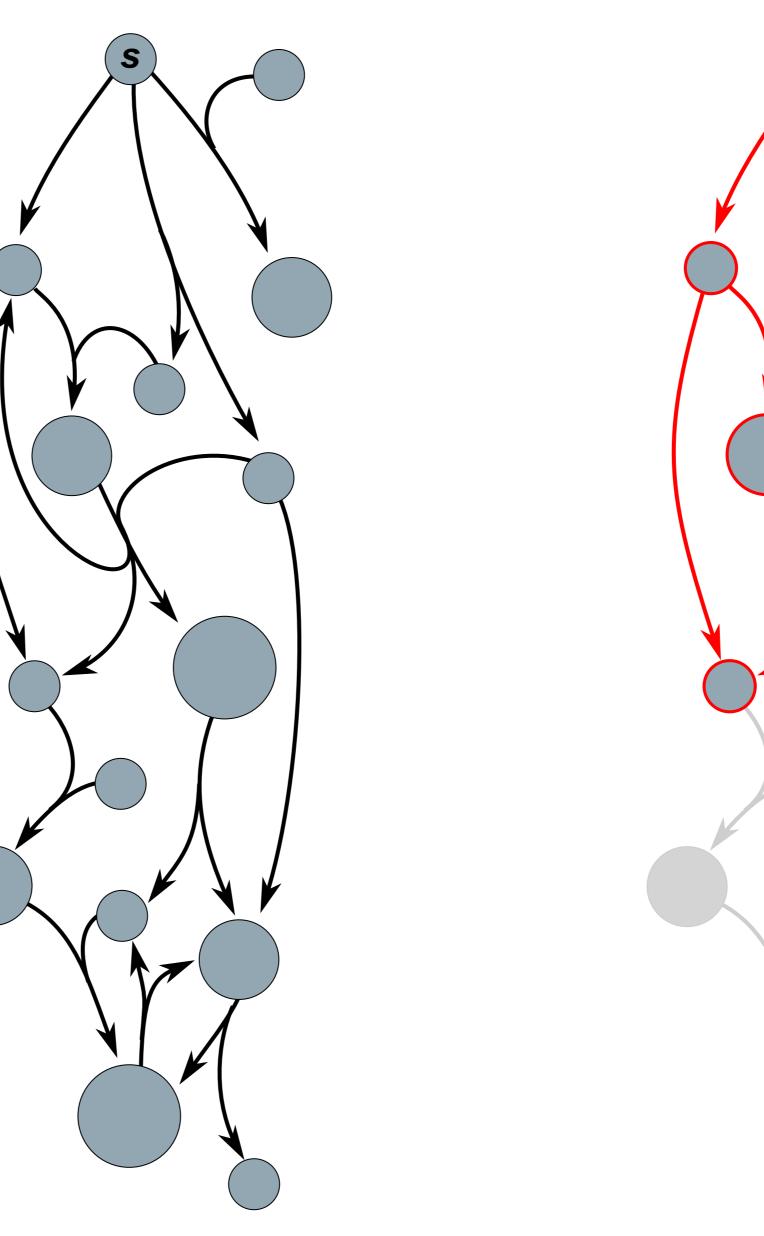
The algorithms currently implemented in *halp* span:

- ► Connectivity [2]
- Hyperpaths [2] [3] [6]
- ► Hypertrees [2]
- ► Random Walks and Partitioning [4] [5]

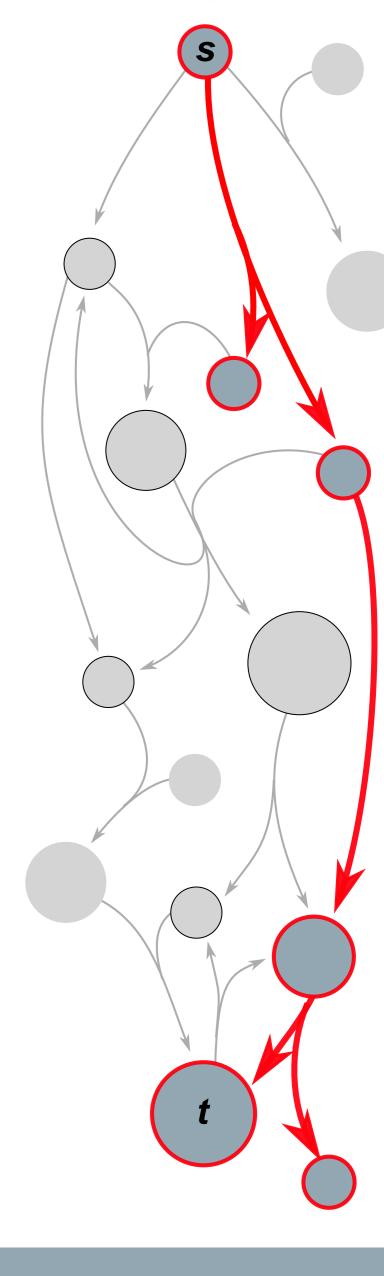
These algorithms are illustrated to the right:

- ► B-Visit algorithm, for computing B-connectivity
- s-t B-hyperpath algorithm, for computing a minimal B-connected hyperpath

Example Algorithms B-Visit from s Initial Hypergraph



s-t B-Hyperpath



New Algorithm with Application to Biological Networks

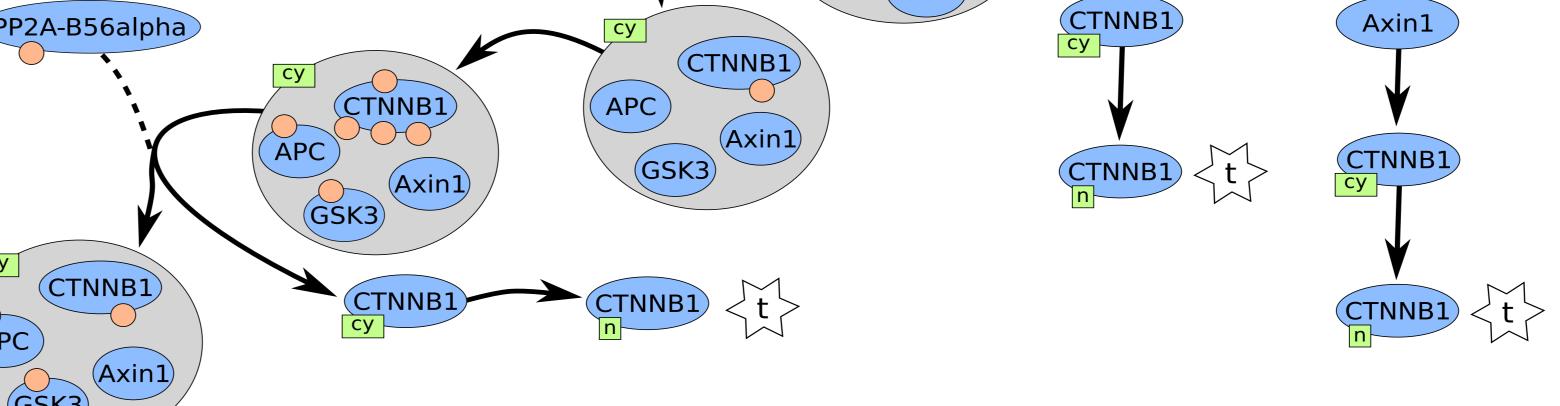
Cellular Signaling Pathways

- Cells respond to environmental signals through "signaling pathways"
- Many types of reactions can occur along these paths
- Graphs cannot model these interactions adequately...but hypergraphs can!

Shortest B-Hyperpath Algorithm

- ► The biological interpretation of a B-hyperpath is a path from node s to node t that contains all intermediate reactants and products needed to reach t from s
- We developed an algorithm using mixed integer linear programming to find the *shortest* acyclic B-hyperpath of all possible B-hyperpaths in a directed hypergraph [6]

Shortest B-Hyperpaths in Signaling Pathways (a) Shortest (b) Shortest Path **B-Hyperpath** (Graph with Complexes) CK1 alpha/epsilon/delta (c) Shortest Path FZD5 (Graph) integral to mem. PP2A-R56alpha



(a) Shortest B-hyperpath in the Wnt signaling pathway when represented as a directed hypergraph.

(b, c) Shortest paths in the Wnt signaling pathway when represented as a graph with complexes (b)

or as a graph (c). We see that the hyperpath is much more informative than the path in the graphs.

Nodes represent complexes (in grey) and standalone proteins (in blue outside of any complexes).

Post-Translational Modification (PTM)

Cellular Compartment Source

Target Hypernode '

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