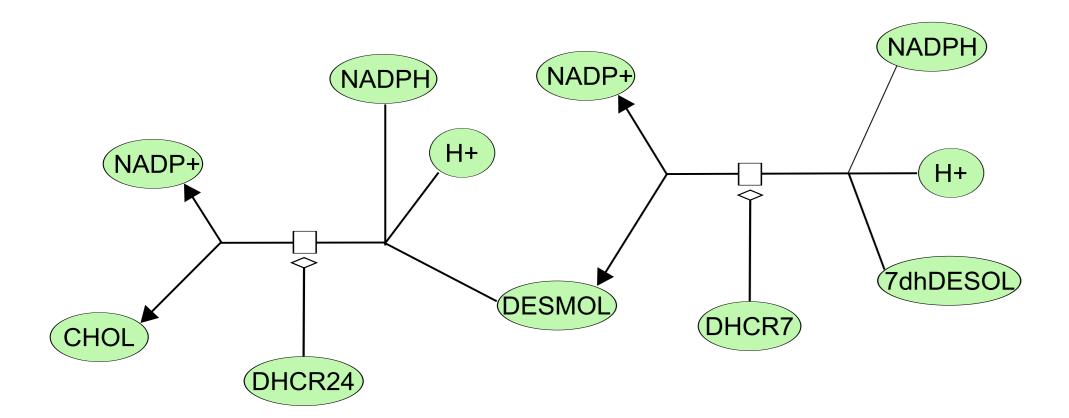
VirginiaTech Invent the Future

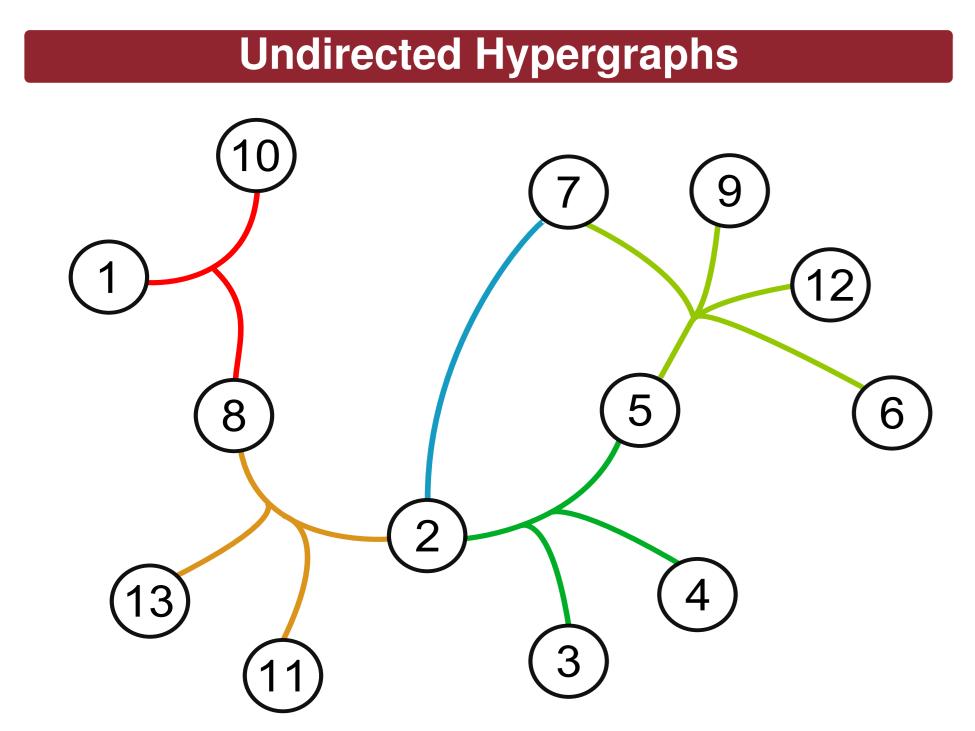
Motivation

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



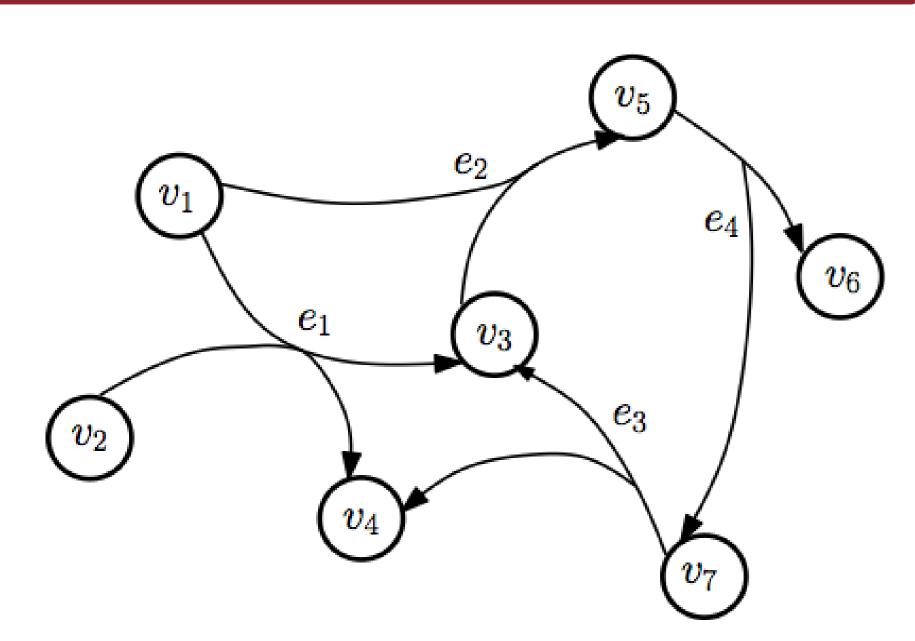
- Many software libraries for graphs exist: NetworkX, Boost, JUNG, etc.
- Challenge: no libraries for hypergraphs exist that have both data structures and algorithms. This leaves a lot of work to do!

What Are Hypergraphs?



Undirected hyperedges connect groups of nodes.

Directed Hypergraphs



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

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

¹Department of Computer Science, Virginia Tech ²ICTAS Center for Systems Biology of Engineered Tissues, Virginia Tech

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

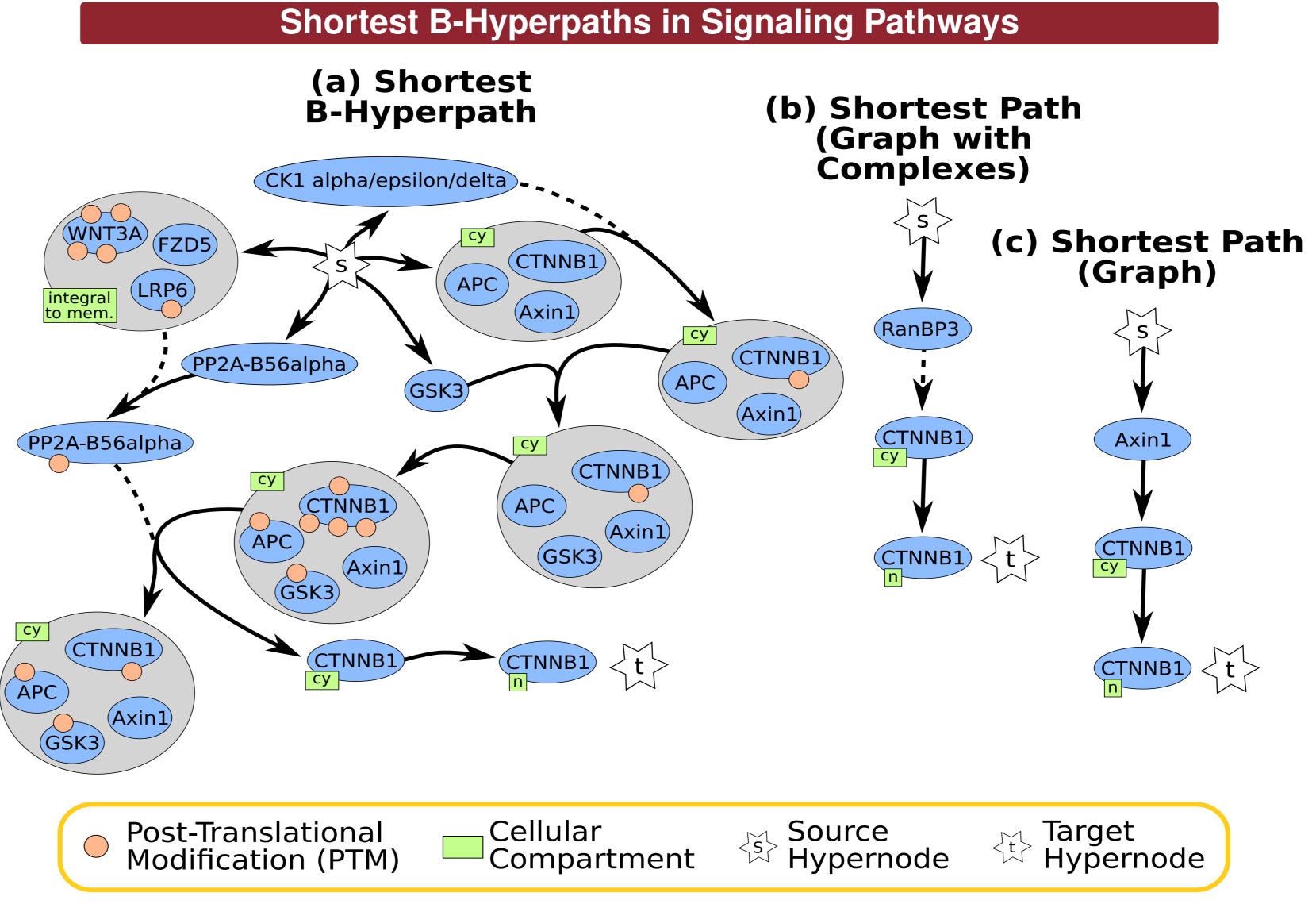
New Algorithm with Application to Biological Networks

Cellular Signaling Pathways

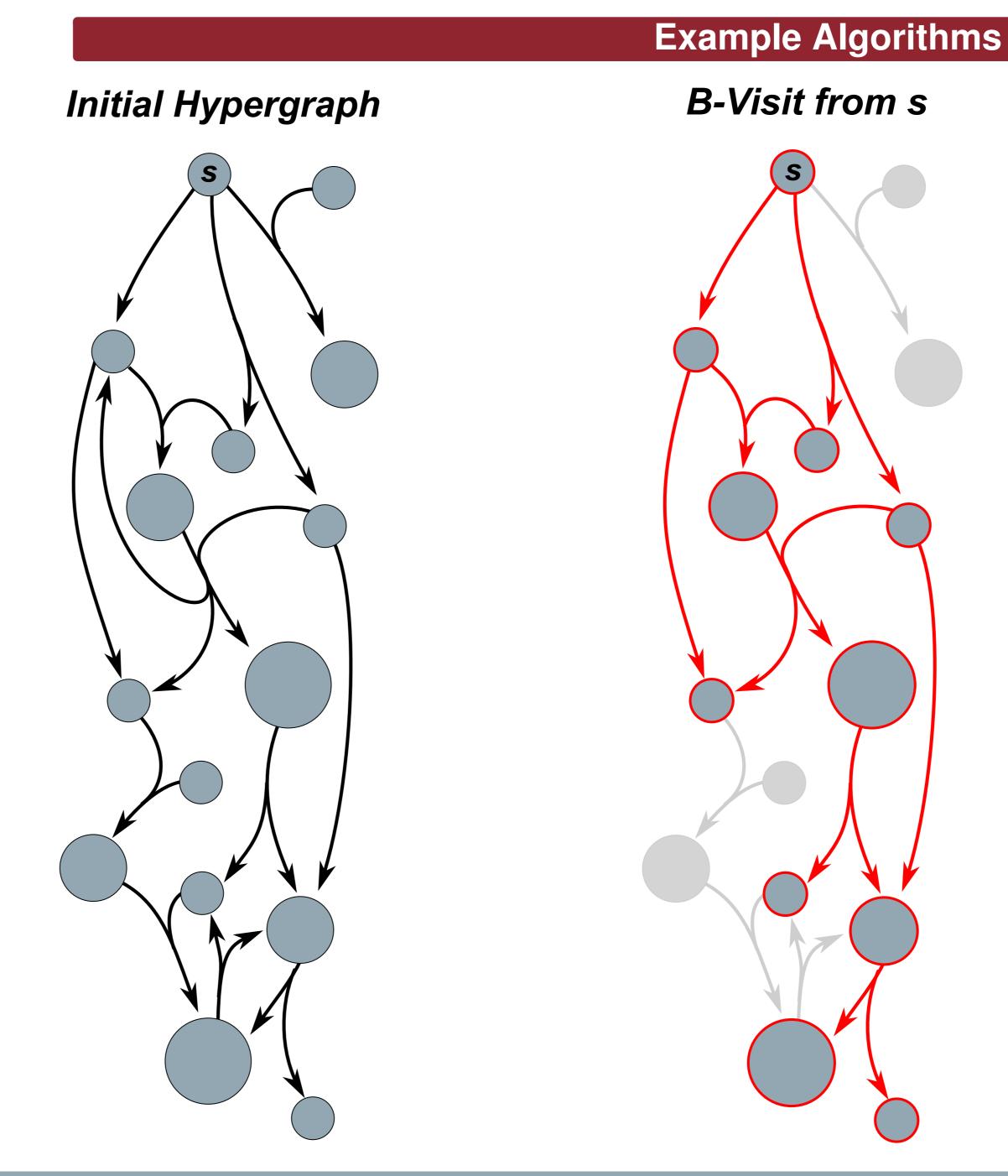
- Cells respond to environmental signals through "signaling pathways"
- Many types of reactions can occur along these paths
- Graphs cannot model these interactions adequately...but hypergraphs can!

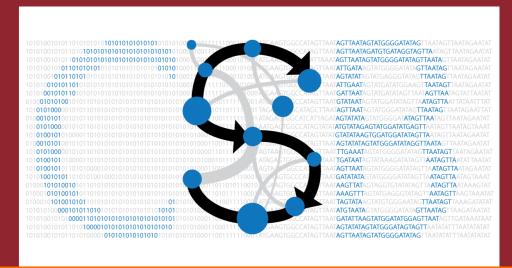
Shortest B-Hyperpath Algorithm

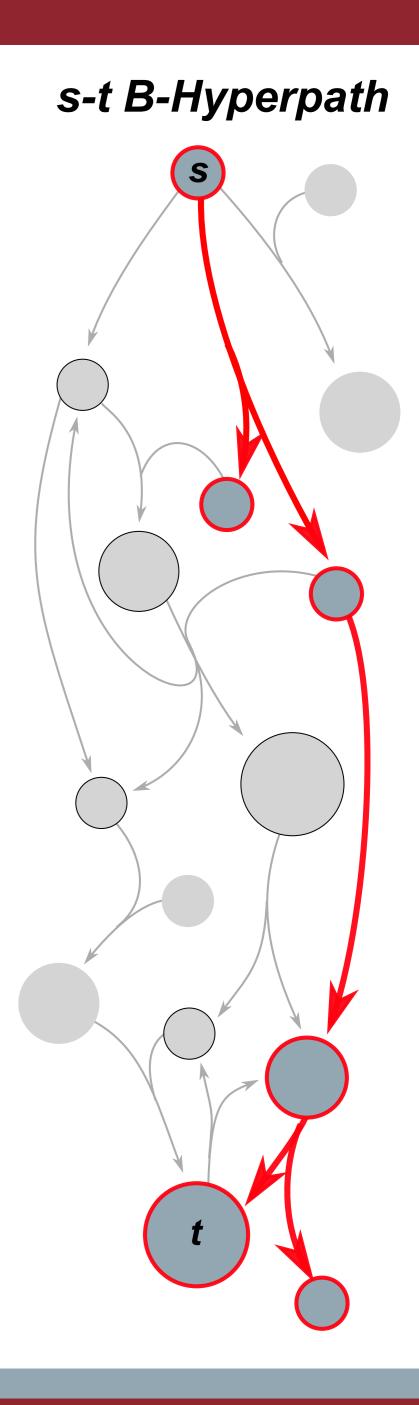
- The biological interpretation of a B-hyperpath is a path from node s to node t that contains all intermediate reactants and products needed to reach t from s
- We developed an algorithm using mixed integer linear programming to find the *shortest* acyclic B-hyperpath of all possible B-hyperpaths in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



(a) Shortest B-hyperpath in the Wnt signaling pathway when represented as a directed hypergraph. Nodes represent complexes (in grey) and standalone proteins (in blue outside of any complexes). (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.







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