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Advantages to Modeling Relational Data using Hypergraphs versus Graphs

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Hypergraph Models for Data Science

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- Explore usage of hypergraphs for modeling complex, multiway (non-pairwise) relational data
- **Goal**: Improve data analysis – more accurate, faster
- **Questions we are trying to address**
  - Why should we use hypergraphs?
  - When are hypergraph models preferable over graph models?
  - What hypergraph model should be used?
  - How should we compute the solution to our hypergraph problems?
- **Specific problem**
  - Data clustering: Determine groupings of data objects given sets of relationships between/amongst objects

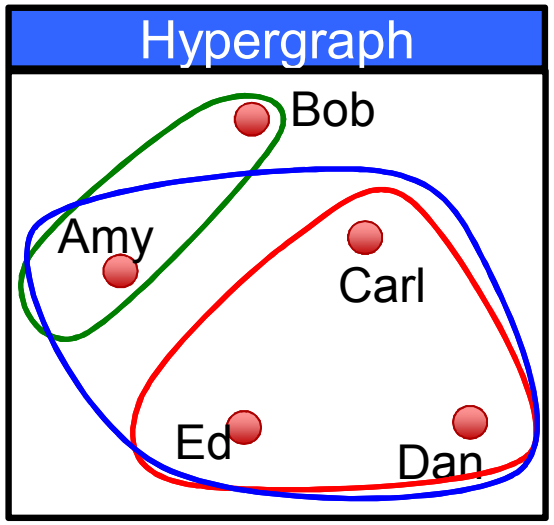
What is a hypergraph?

Hyperedges: Emails

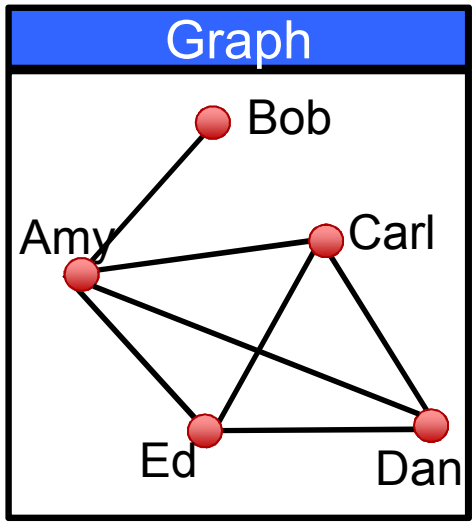
Vertices: Users

	1	2	3
Amy	1		1
Bob	1		
Carl		1	1
Dan		1	1
Ed		1	1

Relational data / hypergraph incidence matrix



Hyperedges connect 1 or more vertices



Edges connect 2 vertices

- Generalizations of graphs
  - Hyperedges represent multiway relationships between vertices
- Convenient representations of relational data
  - Each email (subset of users) can be represented by hyperedge
  - Relational data often stored as hypergraph incidence matrices (e.g., D4M* tables

*Kepner, Jeremy, et al. "Dynamic distributed dimensional data model (D4M) database and computation system." *Acoustics, Speech and Signal Processing (ICASSP), 2012 IEEE International Conference on*. IEEE, 2012.

Hypergraph to Graph: Clique Expansion

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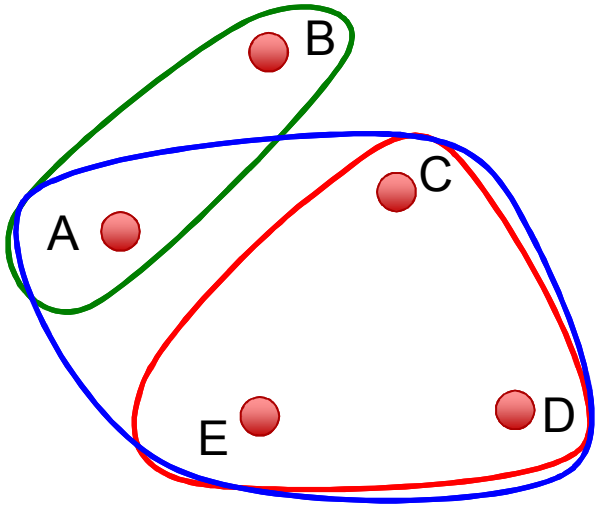
Hyperedges

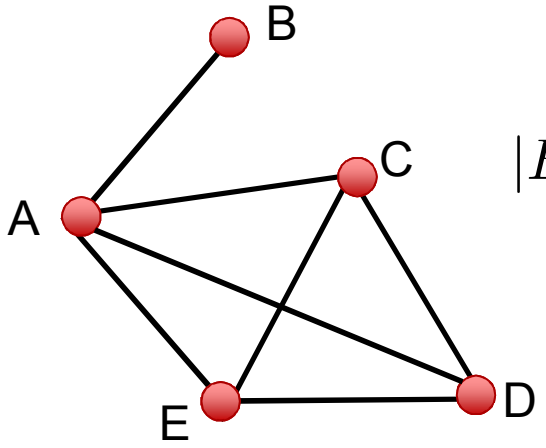
Vertices

	1	2	3
A	1		1
B	1		
C		1	1
D		1	1
E		1	1

Graph Edges

	1	2	3	4	5	6	7	8	9	10
A	1				1	1	1			
B	1									
C		1	1		1			1	1	
D		1		1		1		1		1
E			1	1			1		1	1





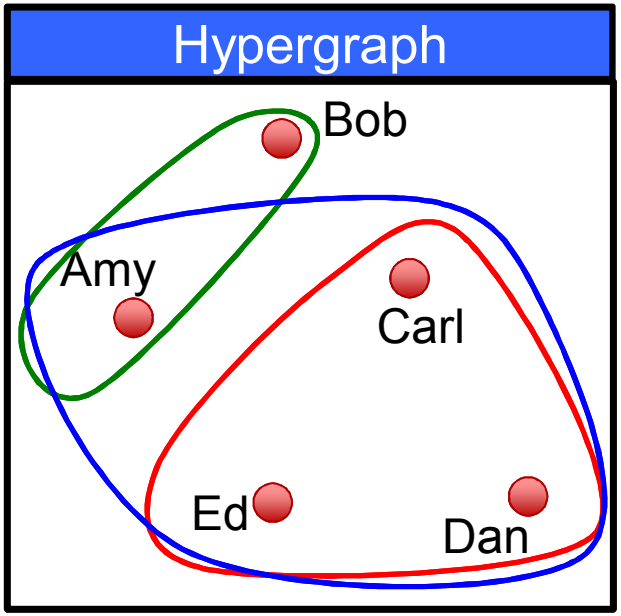
$$|E_g| = \sum_{e_h \in E_h} \binom{d(e_h)}{2}$$

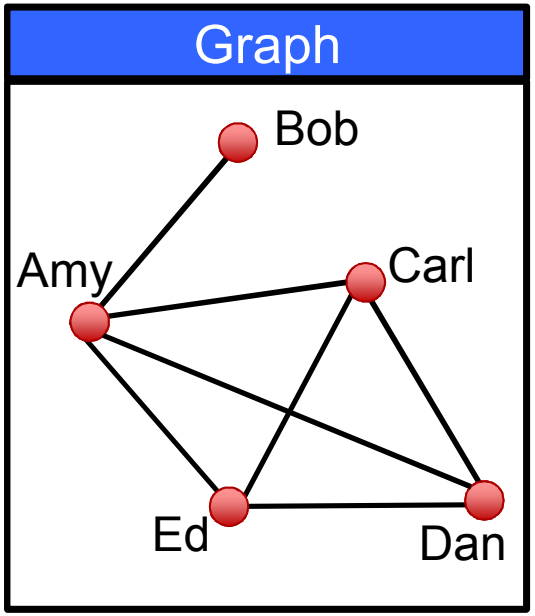
hyperedge cardinality

Graph obtained through clique expansion of hypergraph

Why hypergraphs?

	1	2	3
Amy	1		1
Bob	1		
Carl		1	1
Dan		1	1
Ed		1	1





- Typically graph models lose information
  - Were Carl, Dan, and Ed involved in same email?
  - Fix: multi-graphs + metadata, changes to algorithms

Hypergraphs represent multiway relationships unambiguously

Why hypergraphs?

1		1
1		
	1	1
	1	1
	1	1

Hypergraph incidence matrix

1				1	1	1			
1									
	1	1		1			1	1	
	1		1		1		1		1
		1	1			1		1	1

Graph Incidence matrix

$$|E_g| = \sum_{e_h \in E_h} \binom{d(e_h)}{2}$$

- Hypergraphs require significantly **less storage space** than graphs generated using clique expansion
- Hypergraph incidence matrices require **fewer operations** for matrix-vector multiplication

Hypergraphs have computational advantages

Outline

- Introduction to Hypergraphs
- Spectral clustering
- Software implementation
- Spectral clustering results
- Conclusions

Motivating Problem: Clustering of Relational Data

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- Determine groupings of data objects given sets of relationships amongst those objects
  - Relationships may be represented as graph or hypergraph
- Focus: **spectral clustering**
  - Compute the smallest eigenpairs of the graph or hypergraph Laplacian
  - Normalized graph Laplacian:

$$L_G = I - D_{vG}^{-1/2}(H_G H_G^T - D_{vG})D_{vG}^{-1/2}$$

  - Hypergraph Laplacian (Zhou, et al., 2006)

$$L_h = I - D_{vH}^{-1/2} H_H D_{eH}^{-1} H_H^T D_{vH}^{-1/2}$$

  - Eigenvectors used to group vertices into clusters (sorting, **kmeans++**, …)

SpMV = Sparse matrix-dense vector multiplication

Laplacians: To Form or not to Form

- Laplacians:

$$L_G = I - D_{vG}^{-1/2}(H_G H_G^T - D_{vG})D_{vG}^{-1/2}$$
$$L_h = I - D_{vH}^{-1/2} H_H D_{eH}^{-1} H_H^T D_{vH}^{-1/2}$$

- One option: Explicitly form Laplacian
- Instead: **Define application of Laplacian as series of SpMV and vector addition operations**
  - Store incidence matrix, degree matrices
  - Reason 1: Matrix-matrix products are expensive
  - Reason 2: Dynamic graphs – easier to change incidence matrix than Laplacian

Computational advantages to not explicitly forming Laplacians

SpMV = Sparse matrix-dense vector multiplication

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TriData: Trilinos for Data Analysis

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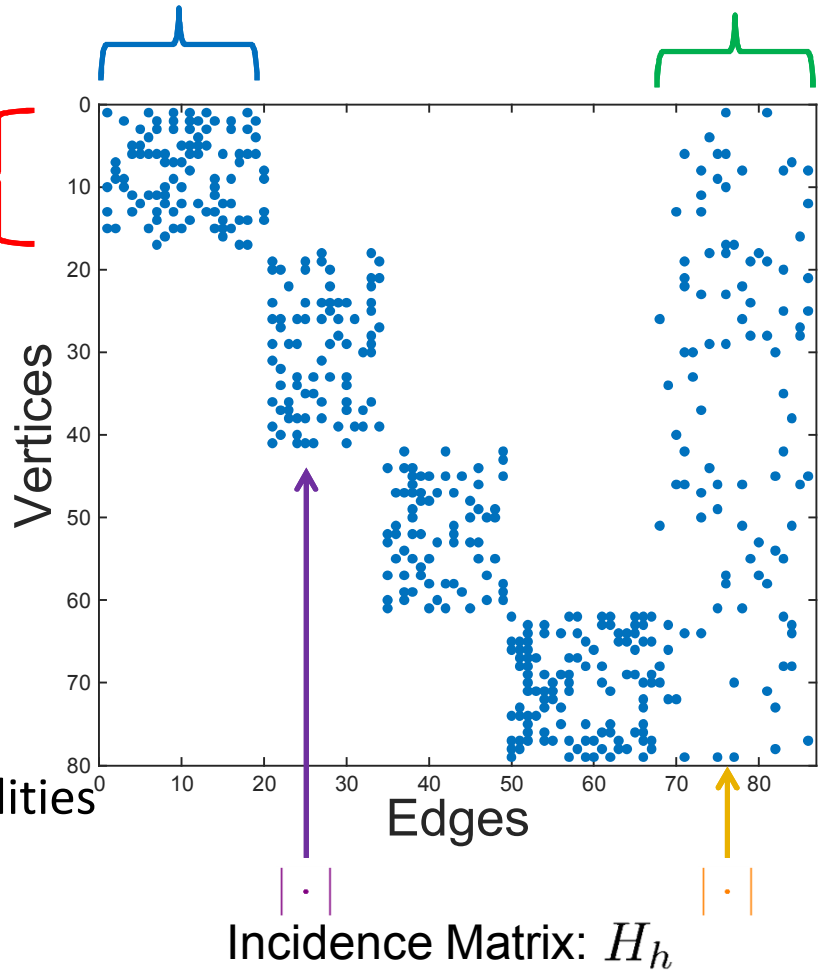
- C++ Trilinos based software for data analytics problems
  - High performance (target: billions of vertices)
  - Early focus on spectral methods
  - Hypergraphs and graphs
- Supports several eigensolvers available in Anasazi
  - LOBPCG, TraceMin-Davidson, Riemannian Trust Region, Block Krylov-Schur
  - Very fast convergence for Laplacians (especially hypergraphs)
- Trilinos/Anasazi supports modern HPC architectures
  - MPI+X
  - Where X = {multicore, GPUs, Xeon Phi…}

Hypergraph Generator

- Randomly generated hypergraphs
  - Stochastic block-like
  - Can generate multiple random instances for each parameter set
- Parameterized Generator
  - Clusters
  - Vertices per cluster
  - # of intra/inter-cluster hyperedges
  - Intra/Inter-cluster hyperedge cardinalities



- **Generate real-world inspired hypergraphs at different scales**
- **Generates "ground truth"**

Outline

- Introduction to Hypergraphs
- Spectral clustering
- Software implementation
- Spectral clustering results
  - Clustering Quality
  - Runtimes
- Conclusions

Numerical Experiments

- Experiments conducted on workstation with 128 GB of memory using 16 cores
- Generated Hypergraphs
  - Number of clusters: 5
  - Vertices per cluster (mean): 10,000
  - Intra/inter-cluster hyperedges (mean): 20,000 / 200,000
  - Intra/inter-cluster hyperedge cardinality (mean): **3-10 / 3-10**
- "Quality" of our clustering measured using the Jaccard index
  - T = true cluster assignments – "ground truth" from generator
  - P = predicted cluster assignments
  - J(T,P)=1 means matches "ground truth" exactly

$$J(T,P) = \frac{|T \cap P|}{|T \cup P|}$$

Outline

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  - Runtimes
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Clustering Quality: Hyperedge Cardinality

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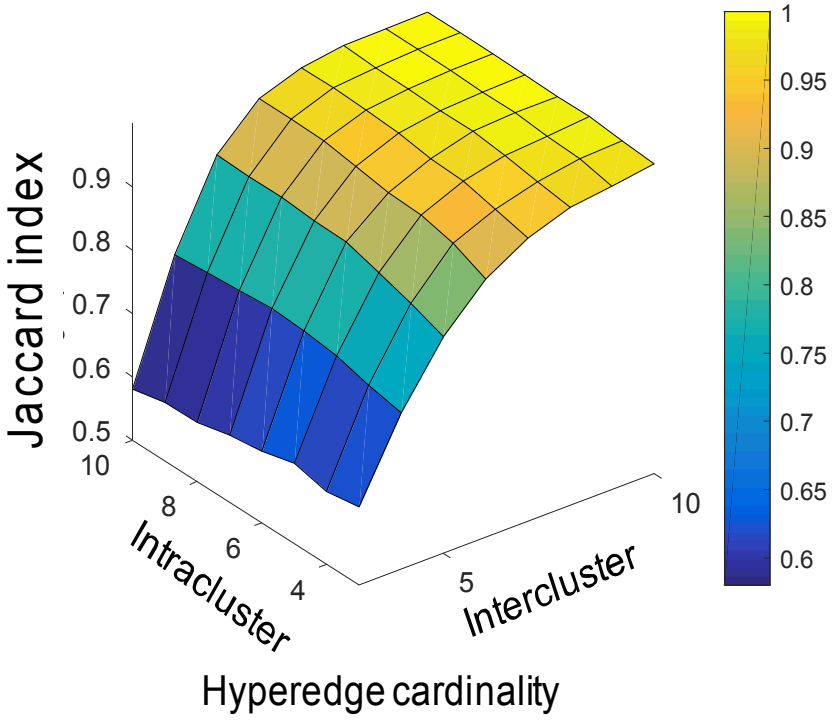
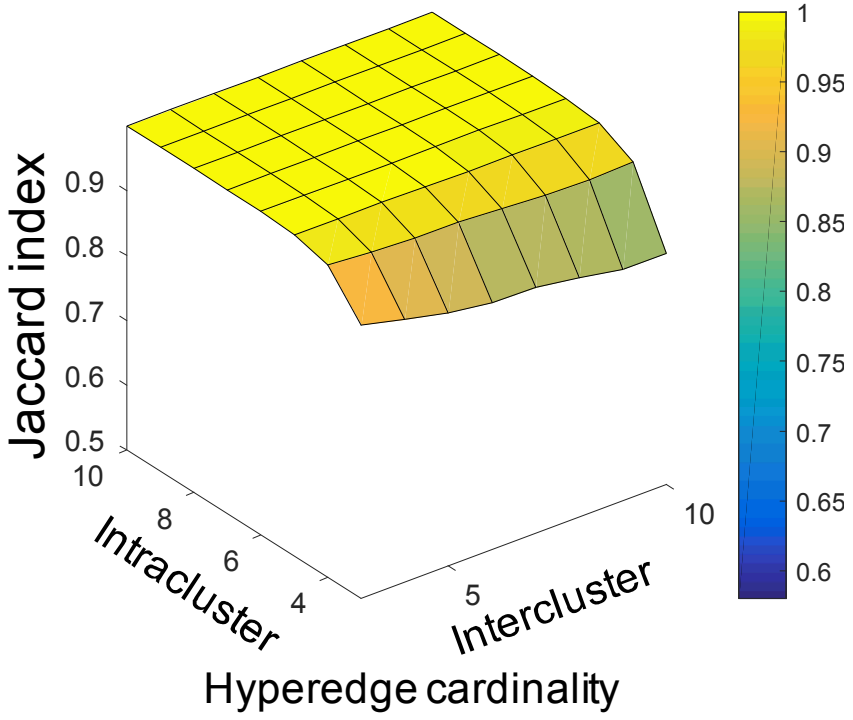
Graph Model



Hypergraph Model



Jaccard Index=1 means clusters match ”ground truth” exactly

General trend: hypergraph based clusters more similar to “ground truth” clusters than graph based clusters

Outline

- Introduction to Hypergraphs
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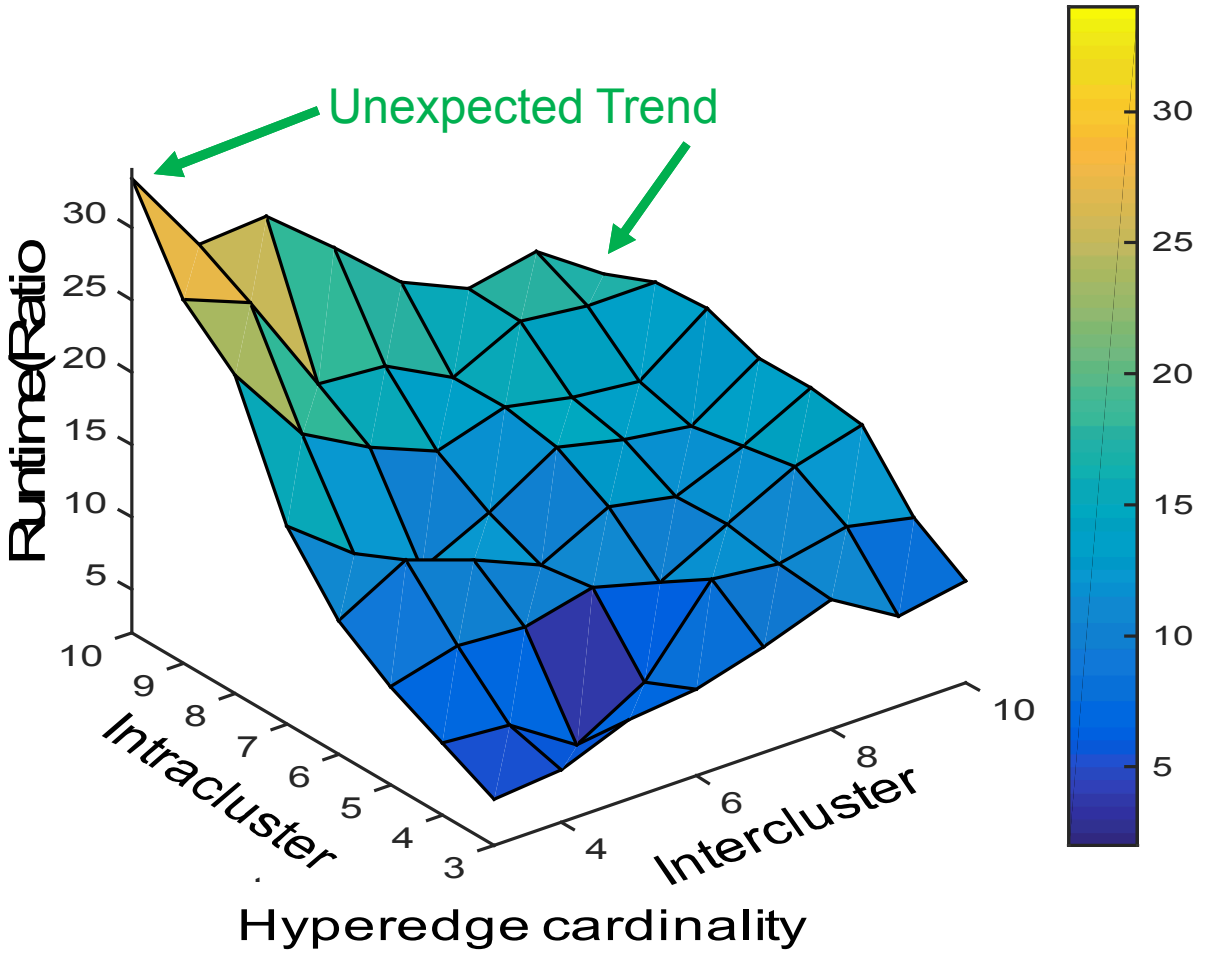
  - Runtimes
- Conclusions

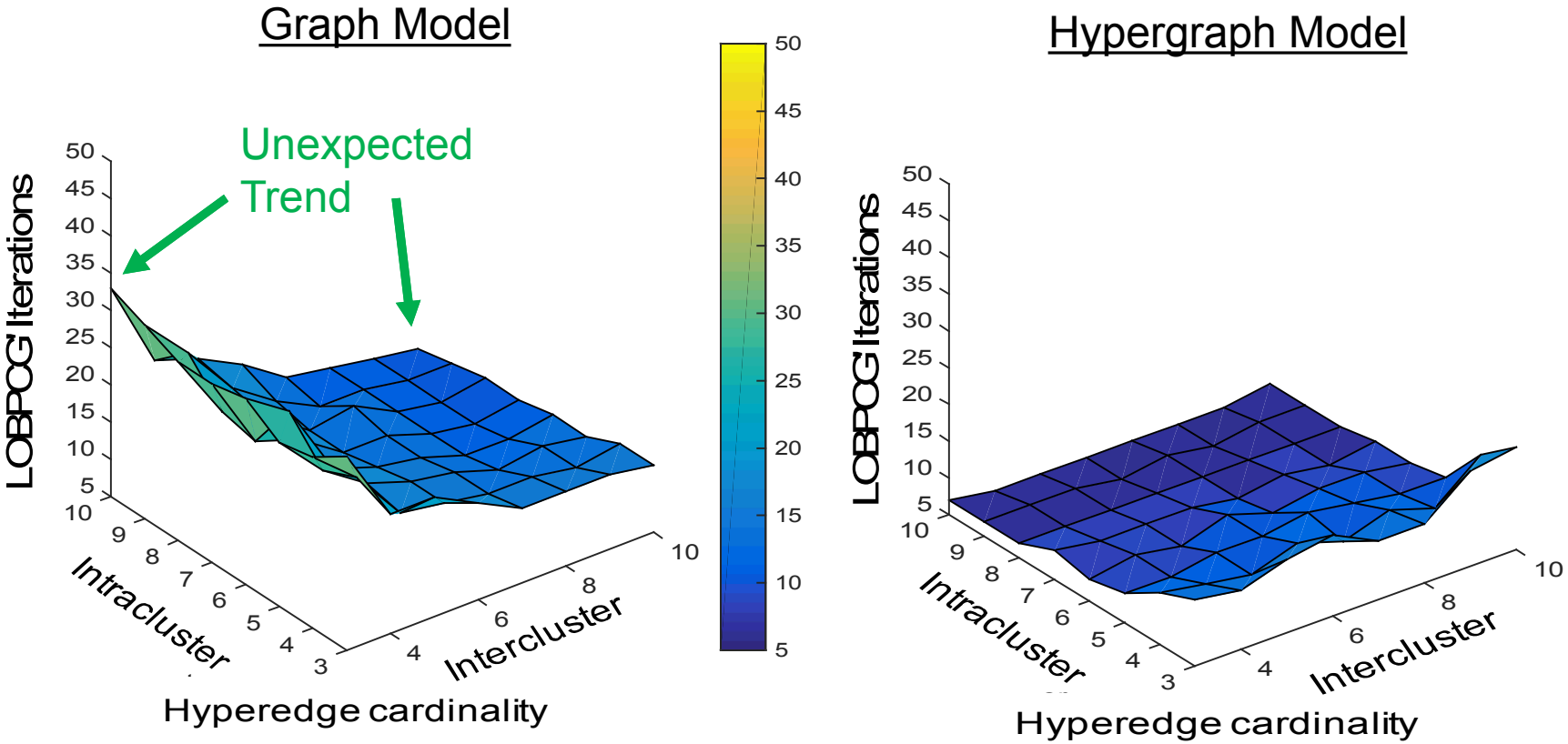
Runtimes: Hyperedge Cardinality



Runtime ratio = graph runtime / hypergraph runtime

Hypergraph models up to 30x faster than graph models

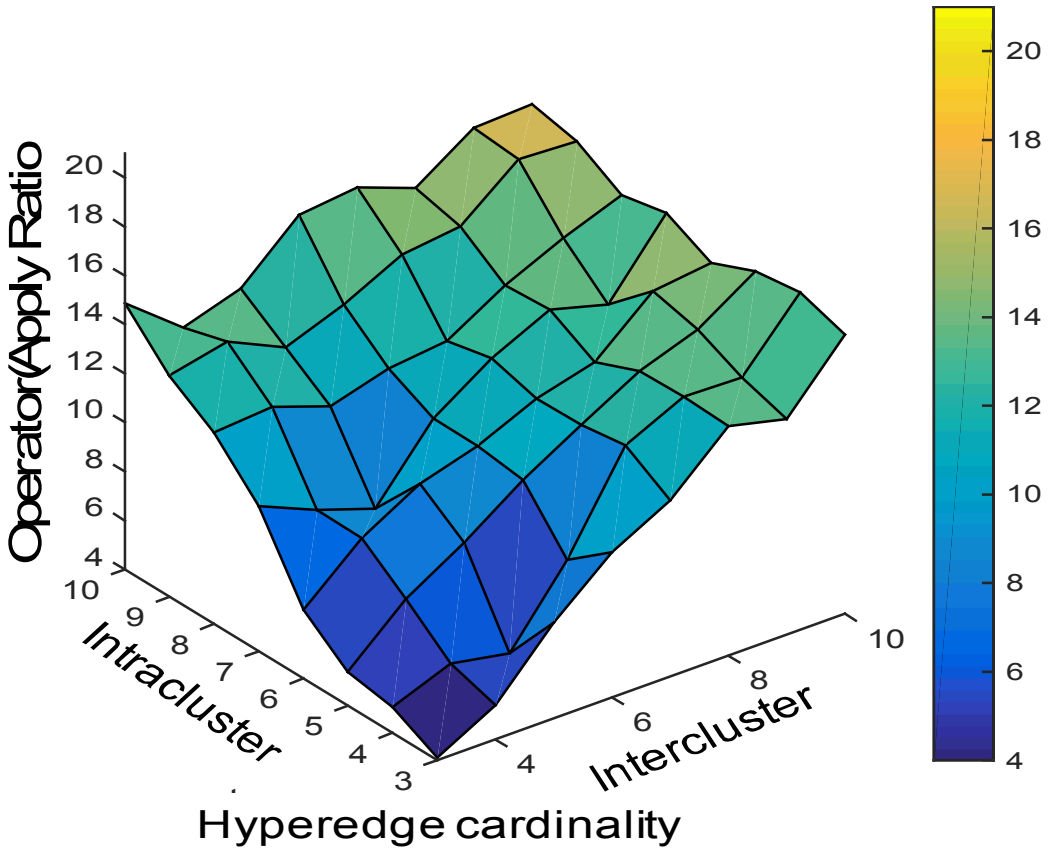
Eigensolver Iterations: Hyperedge Cardinality



- Hypergraph required fewer LOBPCG iterations than graph
  - Better separation of eigenvalues in hypergraph Laplacian

Hypergraph models converged faster (up to 6x) than graph models

Operator Apply Time: Hyperedge Cardinality



Laplacian operator apply more efficient for hypergraph model than graph model (up to 17x faster)

Outline

- Introduction to Hypergraphs
- Spectral clustering
- Software implementation
- Spectral clustering results
- Conclusions

Summary/Conclusions

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- Explored hypergraphs for modeling relational data
  - TriData software for Linear Algebra Based Data Analytics
  - Built on Trilinos framework (target: billions of vertices)
- Compelling advantages for computing on incidence matrices
  - Avoid forming Laplacians, adjacency matrices when possible
- Hypergraphs **extremely** promising for data analytics
  - Better model than graphs for multiway relational data (spectral analysis)
  - **Improvements in quality**
  - **Significant improvements in runtime** (30x)

Future Work

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- Target larger problems
  - Currently solving problems of O(100k) vertices
  - Eventual target: O(1 billion) vertices
- Performance improvements to software
  - 2D partitioning – important for scalability beyond O(10k) processors
  - Improved efficiency of parallel hypergraph generator
- **Promising problems for hypergraphs**: community and anomaly detection; centrality analysis; information propagation; directed hypergraphs for complex, causal relationships

Acknowledgements/References

- Thanks
  - Jon Berry, Rich Lehoucq

- Spectral Clustering
  - Ng, Andrew Y., Michael I. Jordan, and Yair Weiss. "On spectral clustering: Analysis and an algorithm." *Advances in neural information processing systems* 2 (2002): 849-856.
- Hypergraph Laplacian
  - Zhou, Dengyong, Jiayuan Huang, and Bernhard Schölkopf. "Learning with hypergraphs: Clustering, classification, and embedding." *Advances in neural information processing systems*. 2006.
- Related Hypergraph Work
  - Bonacich, Phillip, Annie Cody Holdren, and Michael Johnston. "Hyper-edges and multidimensional centrality." *Social networks* 26.3 (2004): 189-203.
  - Tsuda, Koji. "Propagating distributions on a hypergraph by dual information regularization." *Proc. of 22nd Int. Conf. on Machine learning*. ACM, 2005.
  - Klamt, Steffen, Utz-Uwe Haus, and Fabian Theis. "Hypergraphs and cellular networks." *PLoS Comput Biol* 5.5 (2009): e1000385.

Extra

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What is a hypergraph?

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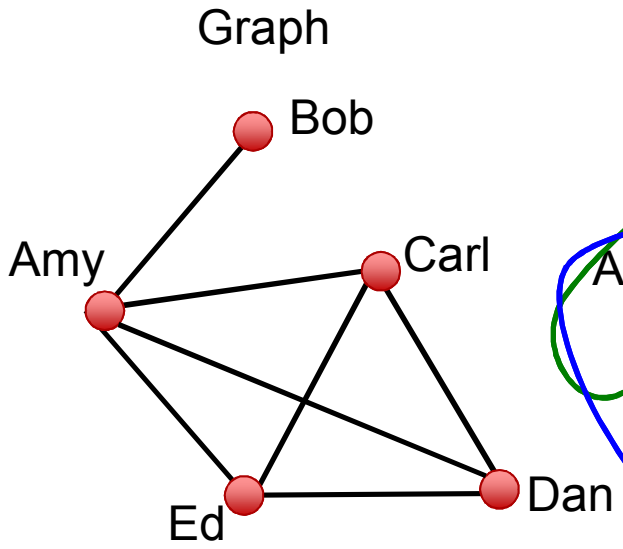
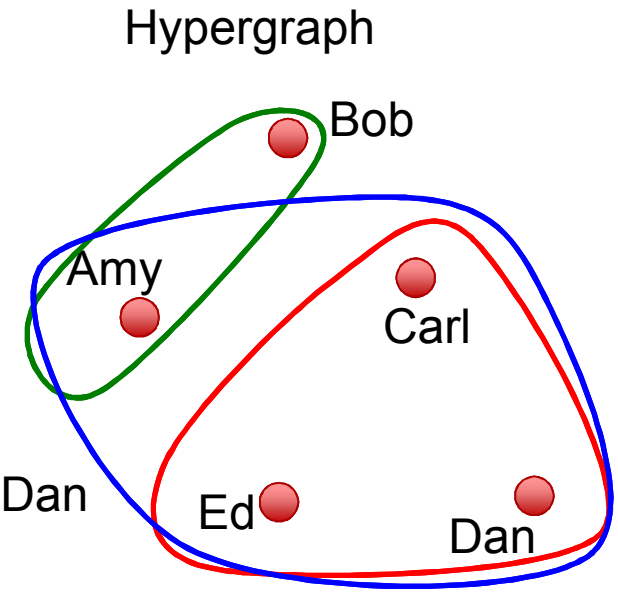
Emails

Users	1	2	3
Amy	x		x
Bob	x		
Carl		x	x
Dan		x	x
Ed		x	x

Relational Data





- Convenient representation of relational data
  - Each email can be represented by hyperedge
  - Emails/hyperedges consist of subsets of users

What is a hypergraph?

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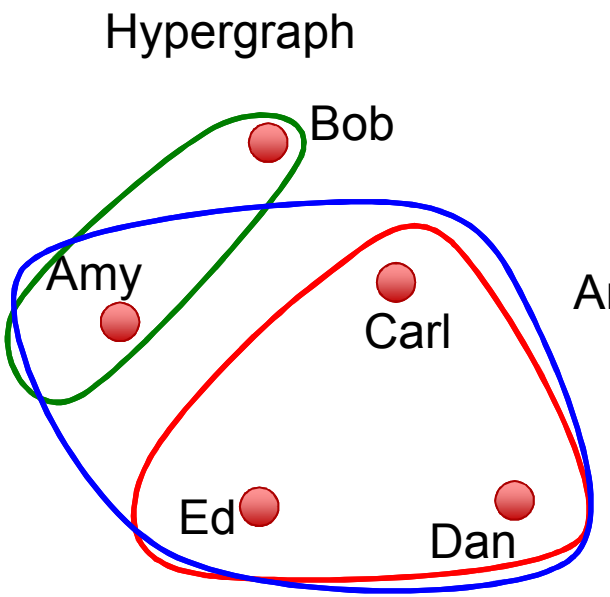
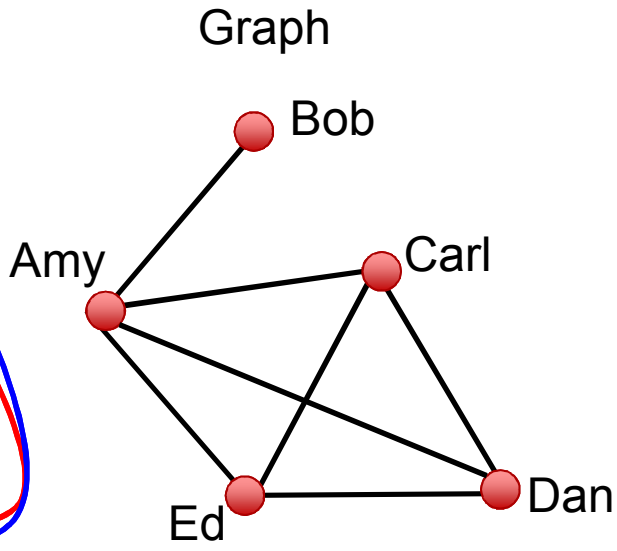
Hyperedges: Emails

Vertices: Users

	1	2	3
Amy	1		1
Bob	1		
Carl		1	1
Dan		1	1
Ed		1	1

Hypergraph incidence matrix





- Relational data is often stored as hypergraph incidence matrix
  - E.g., D4M* tables
- Graph obtained through clique expansion of hypergraph

*Kepner, Jeremy, et al. "Dynamic distributed dimensional data model (D4M) database and computation system." *Acoustics, Speech and Signal Processing (ICASSP), 2012 IEEE International Conference on*. IEEE, 2012.

Hypergraph clique expansion

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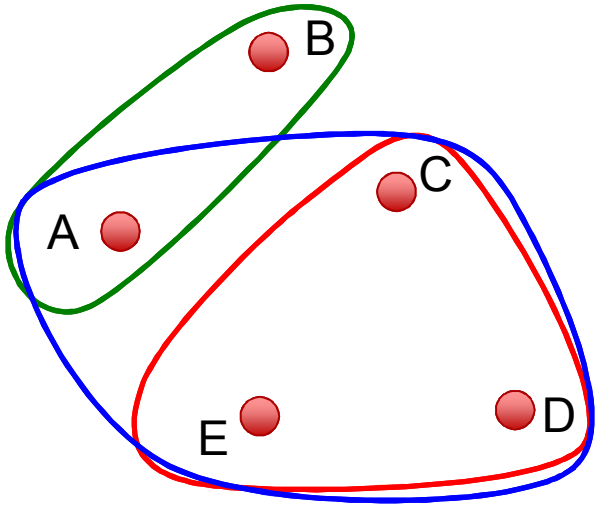
Hyperedges

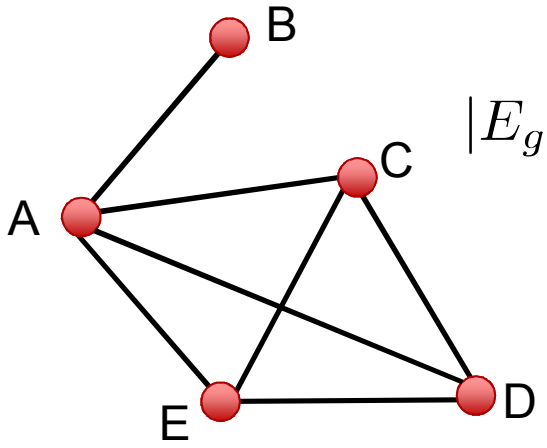
Vertices

	1	2	3
A	1		1
B	1		
C		1	1
D		1	1
E		1	1

Graph Edges

	1	2	3	4	5	6	7	8	9	10
A	1				1	1	1			
B	1									
C		1	1		1			1	1	
D		1		1		1		1		1
E			1	1			1		1	1





$$|E_g| = \sum_{e_h \in E_h} \binom{d(e_h)}{2}$$

hyperedge cardinality

Weighted hypergraph clique expansion

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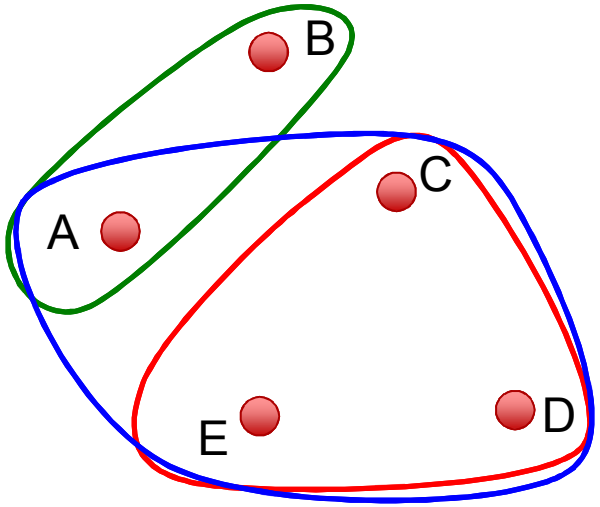
Hyperedges

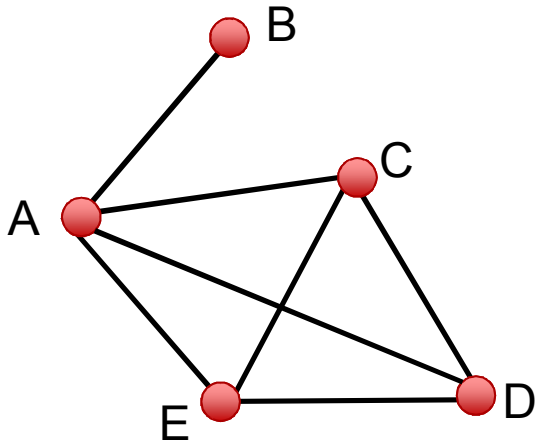
Vertices

	1	2	3
A	1		1
B	1		
C		1	1
D		1	1
E		1	1

Graph Edges

	1	2	3	4	5	6	7	8	9	10
A	1				⅓	⅓	⅓			
B	1									
C		½	½		⅓			⅓	⅓	
D		½		½		⅓		⅓		⅓
E			½	½			⅓		⅓	⅓





$$w(e_g) = \frac{1}{d(e_h) - 1}$$

hyperedge cardinality

Motivating Problem: Clustering Relational Data

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- Determine groupings of data objects given sets of relationships amongst those objects
- Relationships may be represented as graph or hypergraph
  - Graphs represent pairwise relationships
  - Hypergraphs represent relationships among groups of things
- Applications
  - Finding emerging research trends from documents (Jung et al., 2014)
  - Clustering categorical data (Gibson et al., 2000)
  - Image segmentation (Agarwal et al., 2005)
  - Metabolic networks (Guimera et al., 2004)

Related Hypergraph Work

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- Data partitioning (Computational science & engineering)
  - Circuit layout, parallel processing, …
- Hypergraph eigencentrality (Bonacich, et al., 2004)
  - Analysis of attacks on Caribbean settlements
- Semi-supervised Learning (Tsuda, 2005)
  - Information propagation across hypergraph, prior knowledge
- Biological networks (Klamt, et al., 2009)
  - Biochemical reactions, finding related proteins (functional groups)

- Caveat emptor – hypergraphs
  - Representations may increase complexity of algorithms (e.g., MST)
  - Avoid such problems

Unweighted graph vs hypergraph clustering

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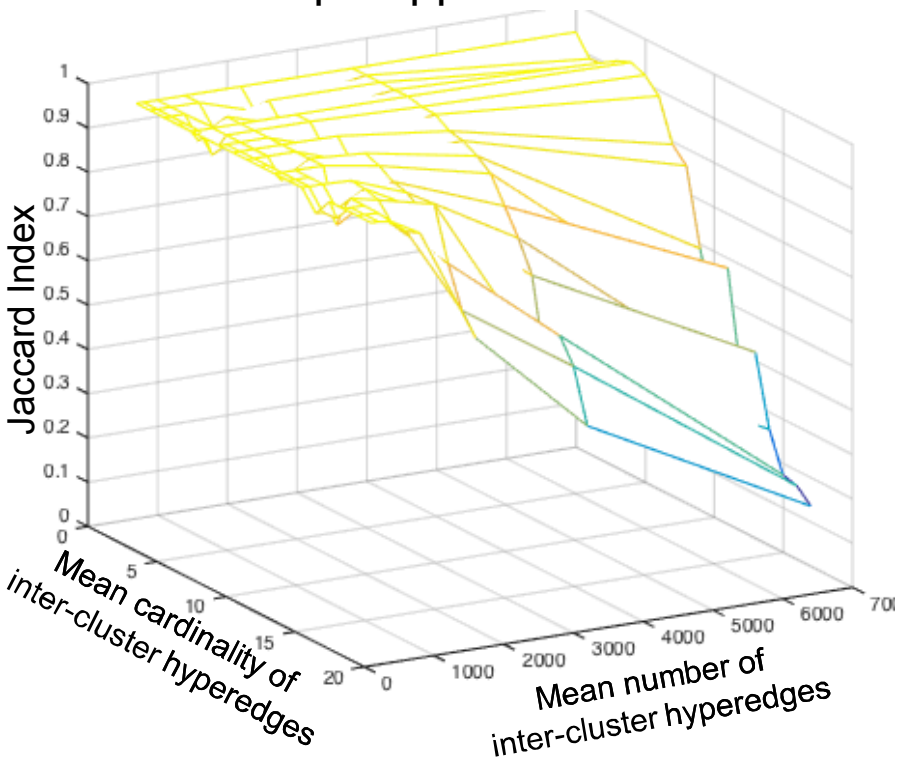
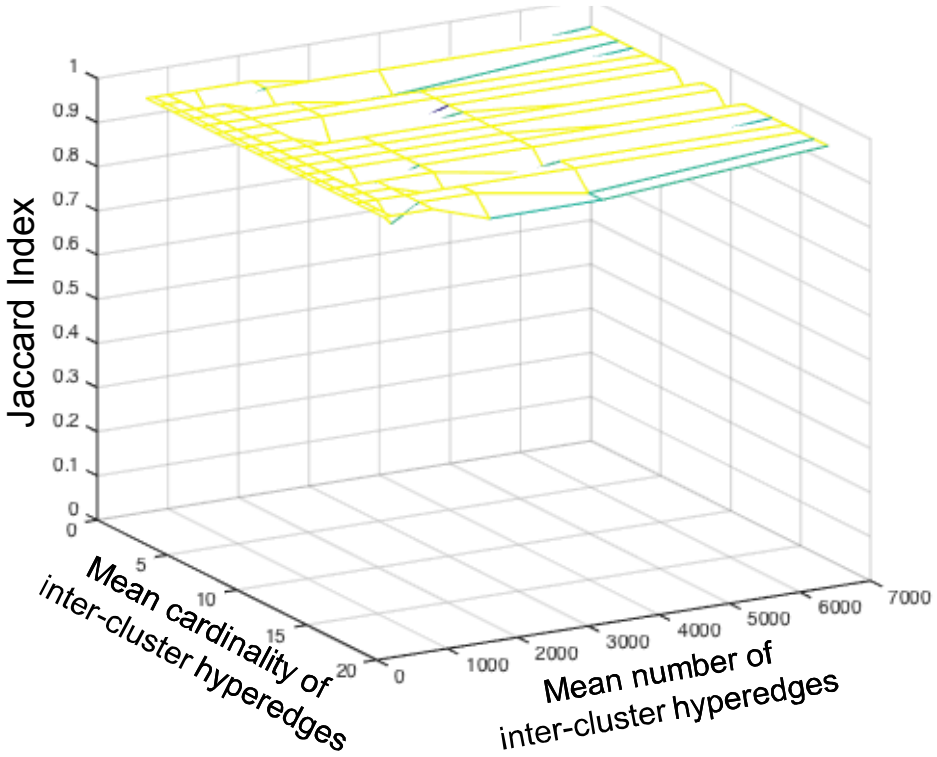
Graph Approach



Hypergraph Approach



Mean intra-cluster cardinality = 3
Number of clusters 4, mean size 100
Mean number of inter-cluster edges: 800

Weighted graph vs hypergraph clustering

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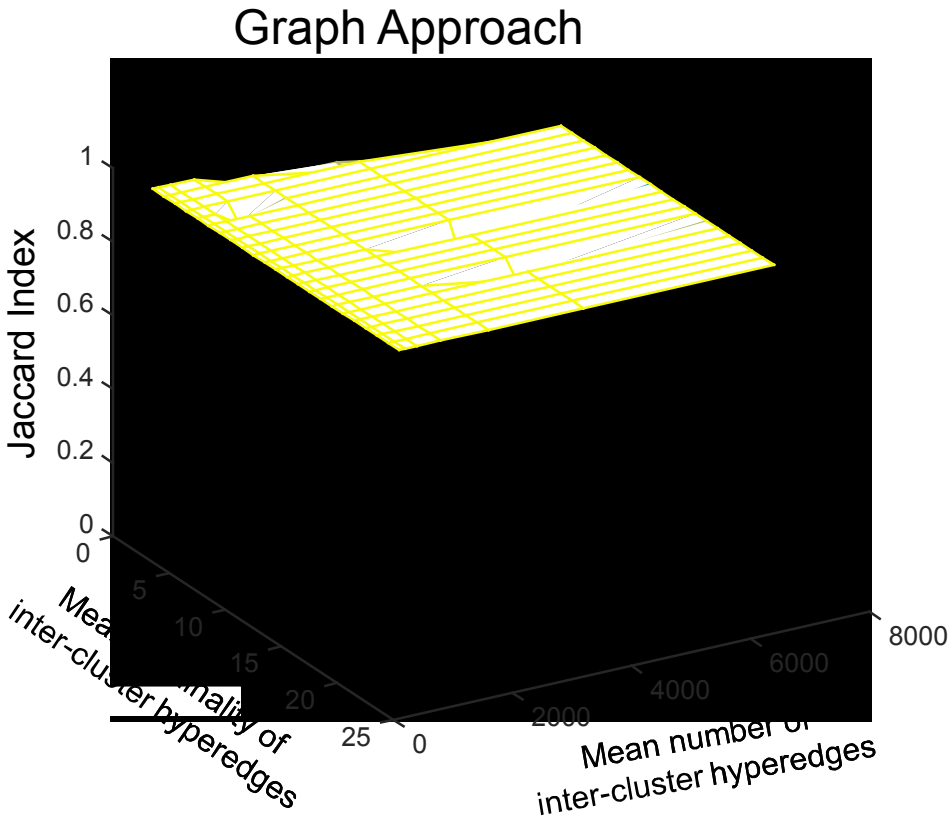

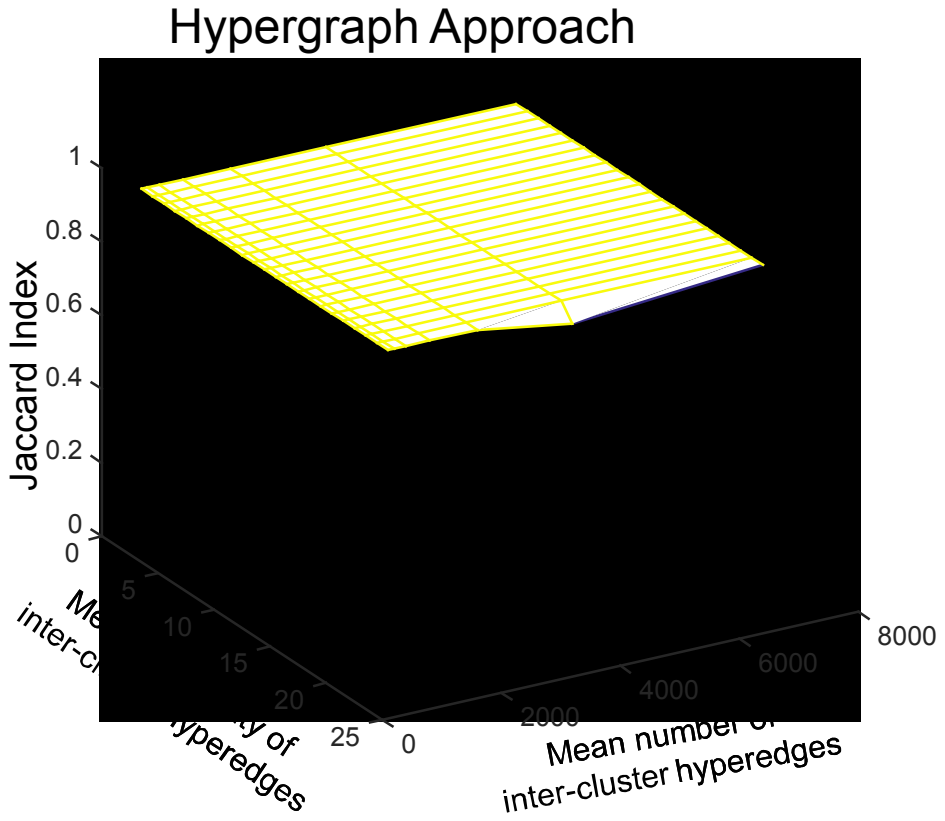

Number of clusters = 4
Mean number of vertices = 100
Number of eigenvectors = 5

Plot of eigenvalues

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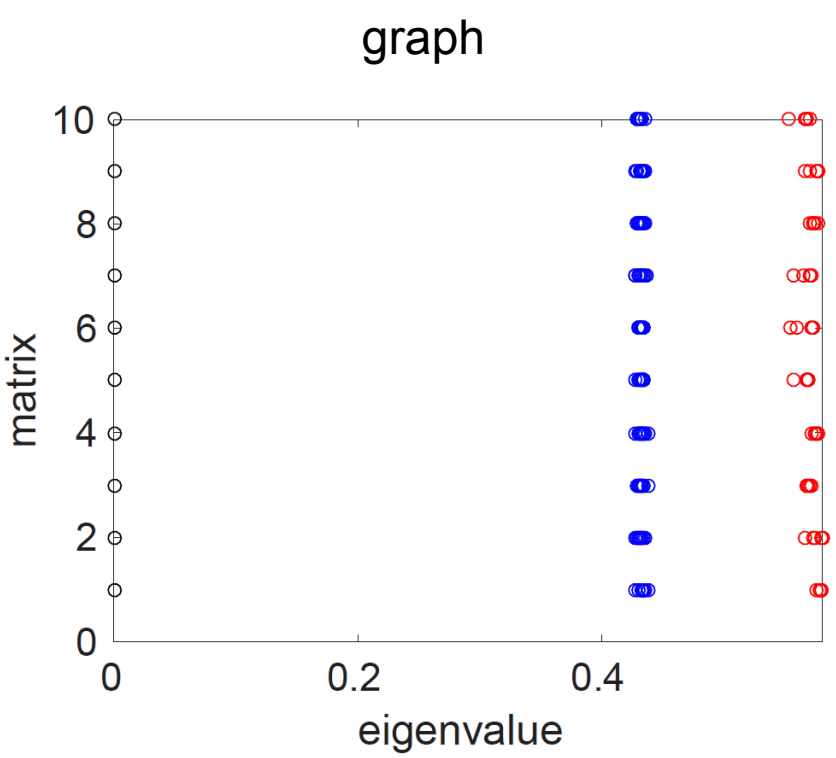
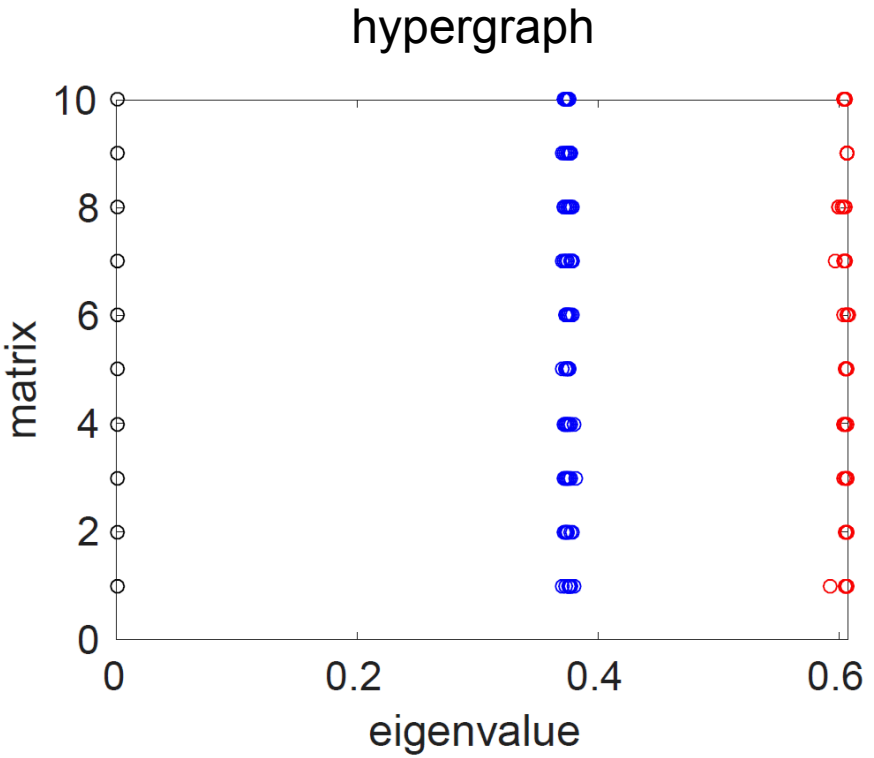
P3





Number of clusters	10
Nodes per cluster	10,000
Intra/Inter-cluster hyperedges	20,000 200,000
Intra/Inter-cluster h-edge cardinality	5 5

Formulation of the eigenvalue problem

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- Computing the smallest eigenpairs of

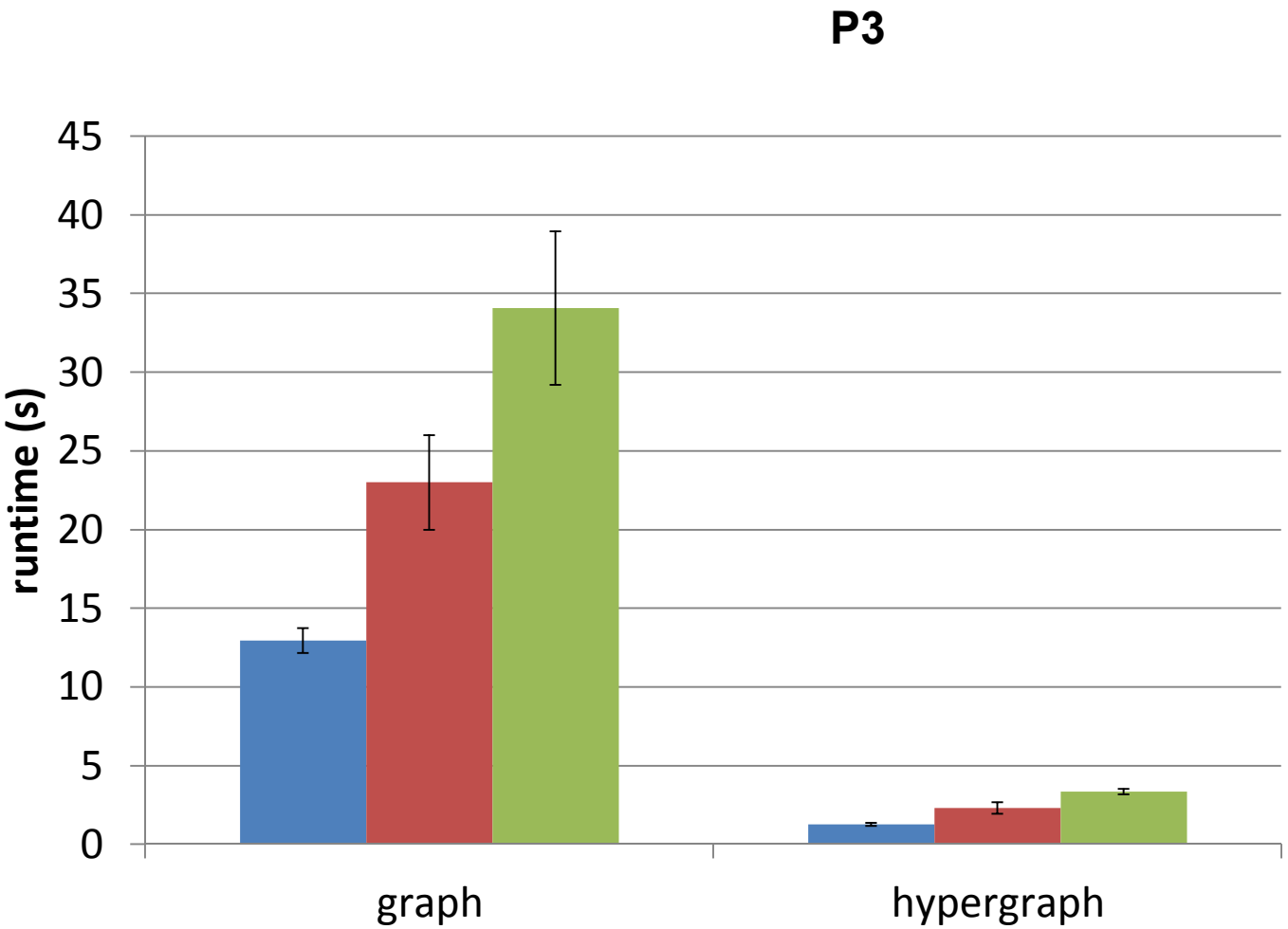
$$L_G = I - D_{vG}^{-1/2}(H_G H_G^T - D_{vG})D_{vG}^{-1/2} \qquad L_h = I - D_{vH}^{-1/2} H_H D_{eH}^{-1} H_H^T D_{vH}^{-1/2}$$

  is equivalent to computing the largest eigenpairs of the shifted Laplacians

$$S_G = D_{vG}^{-1/2}(H_G H_G^T - D_{vG})D_{vG}^{-1/2} \qquad S_h = D_{vH}^{-1/2} H_H D_{eH}^{-1} H_H^T D_{vH}^{-1/2}$$

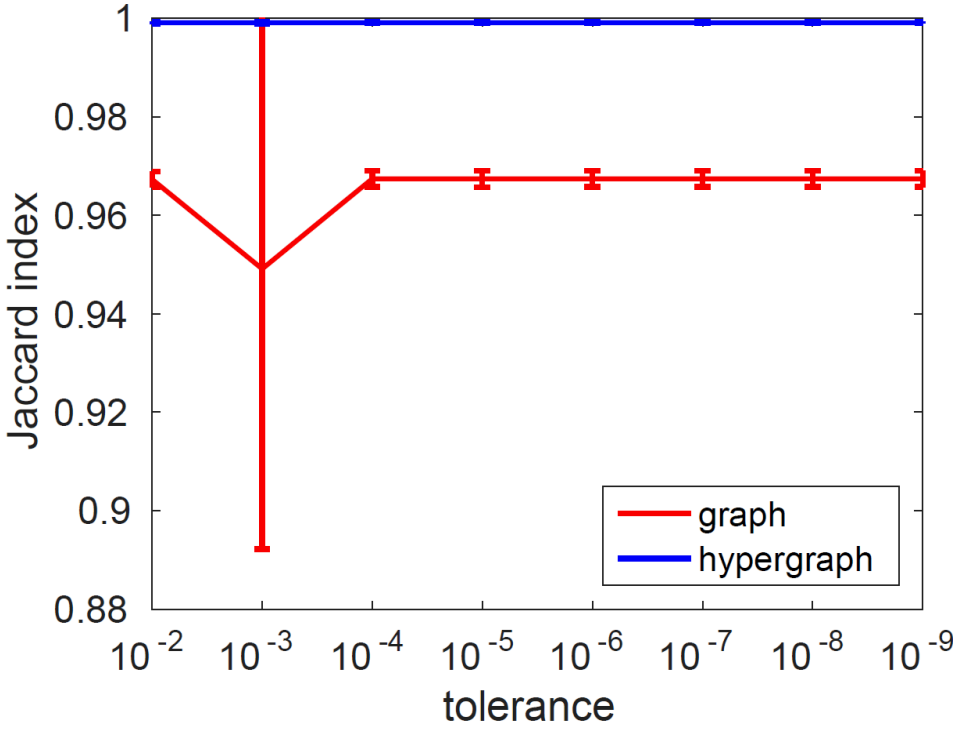
  - Computing the largest eigenpairs tends to be cheaper
  - Laplacians are singular (but null space is known)
  - L_g, L_h, and S_h are symmetric positive definite, but S_g is not
  - S_g can be shifted even more to make it positive definite

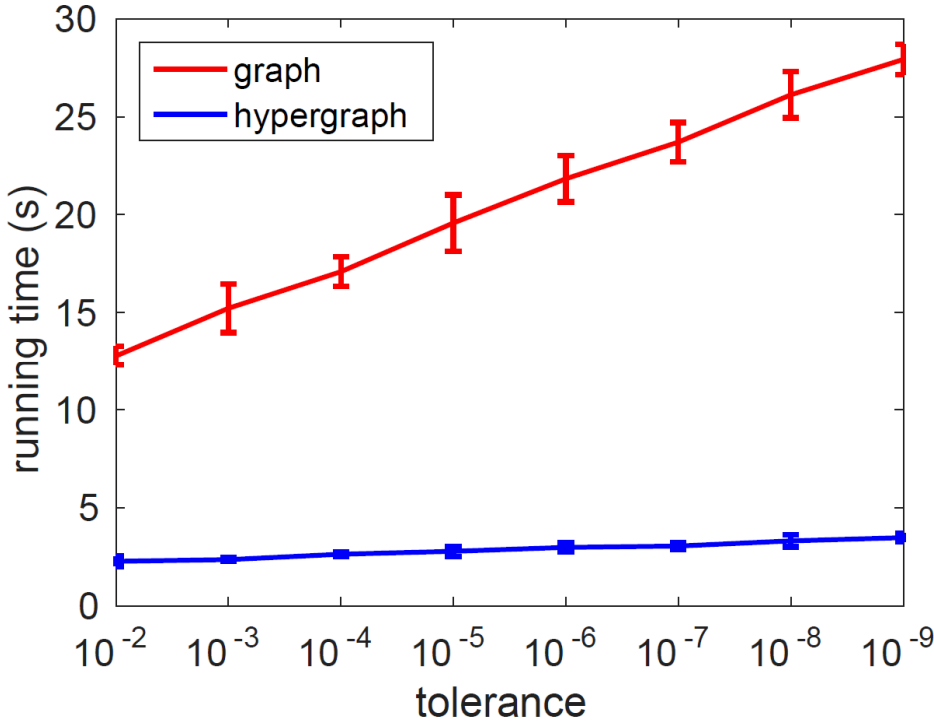
Comparison of eigensolvers



Number of clusters	10
Nodes per cluster	10,000
Intra/Inter-cluster hyperedges	20,000 200,000
Intra/Inter-cluster h-edge cardinality	5 5

What tolerance should we use?

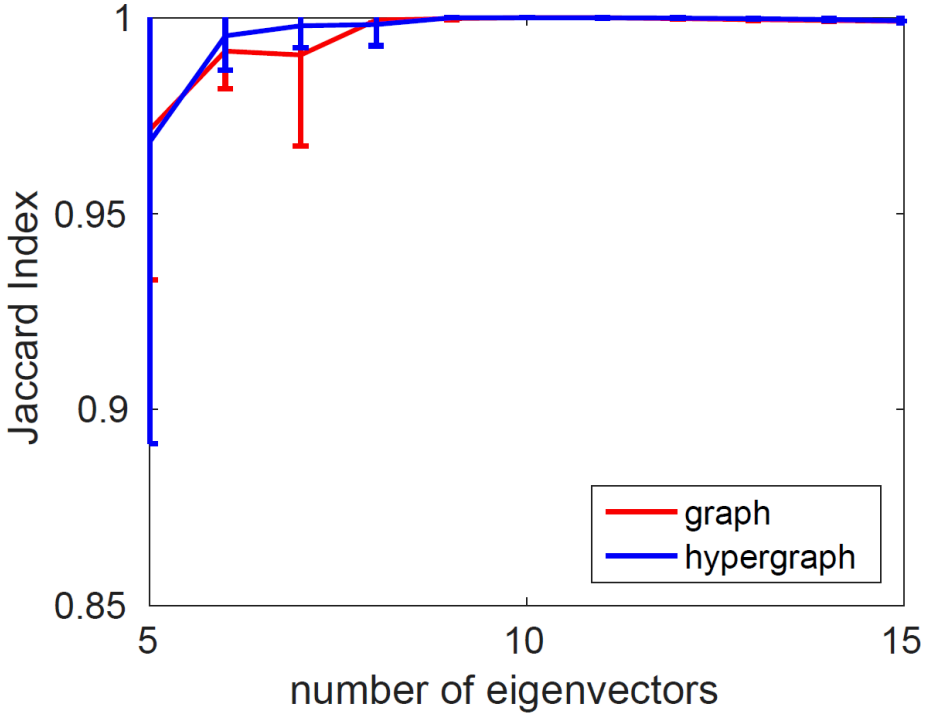


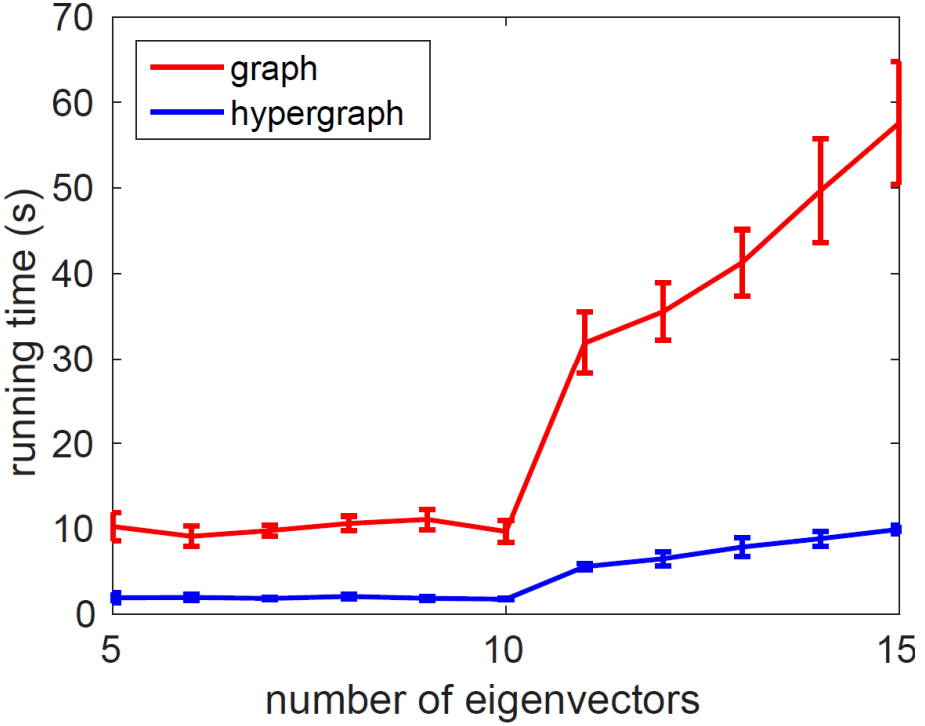


P3

Number of clusters	10
Nodes per cluster	10,000
Intra/Inter-cluster hyperedges	20,000 200,000
Intra/Inter-cluster h-edge cardinality	5 5

How many eigenvectors should we calculate?

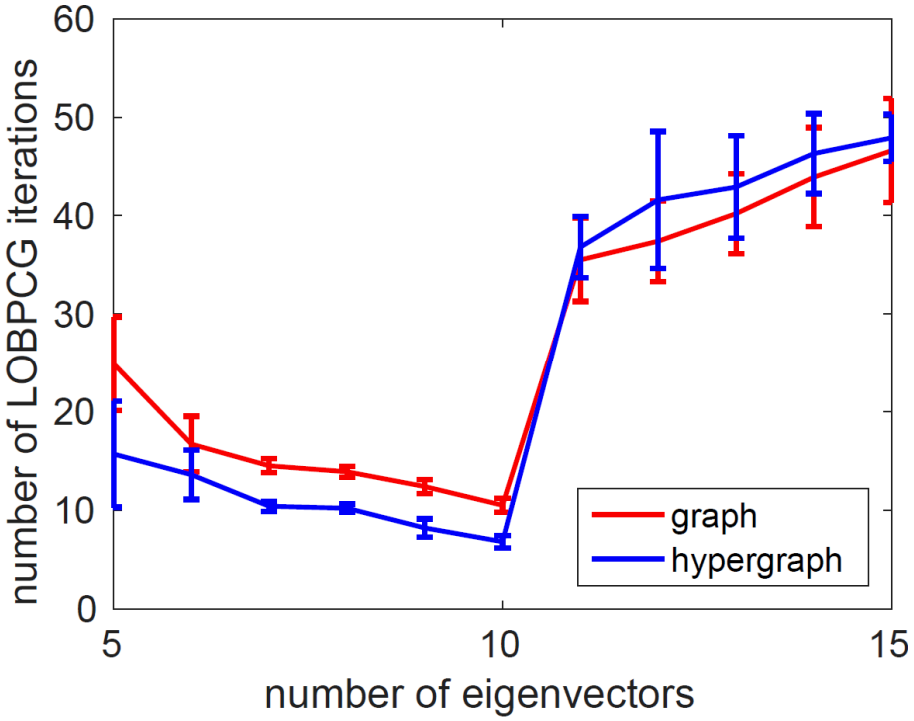




Less noisy data: P1

Number of clusters	10
Nodes per cluster	10,000
Intra/Inter-cluster hyperedges	40,000 50,000
Intra/Inter-cluster h-edge cardinality	5 5

How many eigenvectors should we calculate?



Less noisy data: P1

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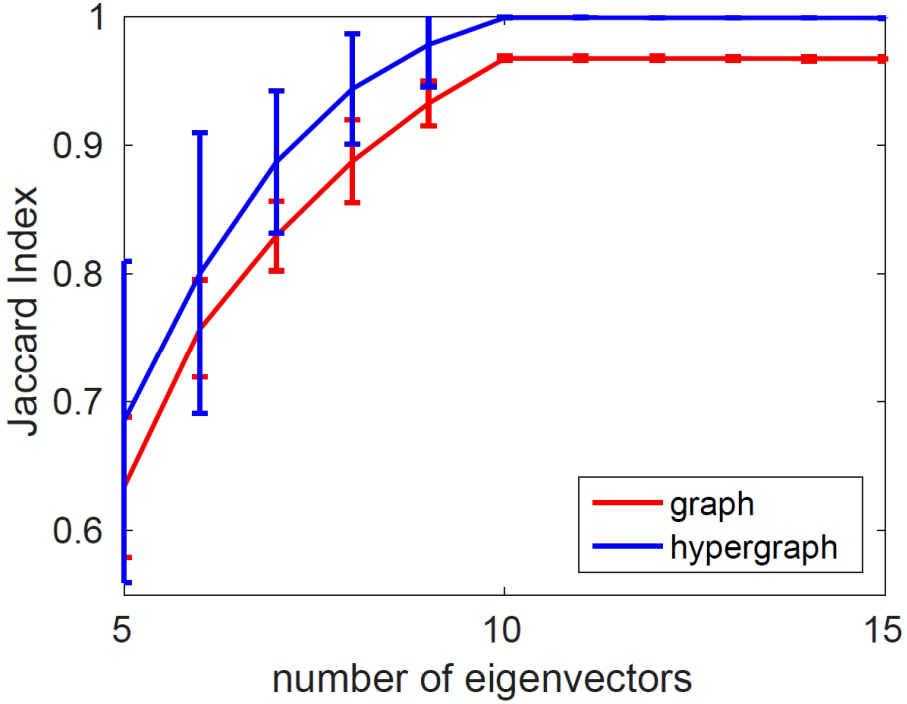
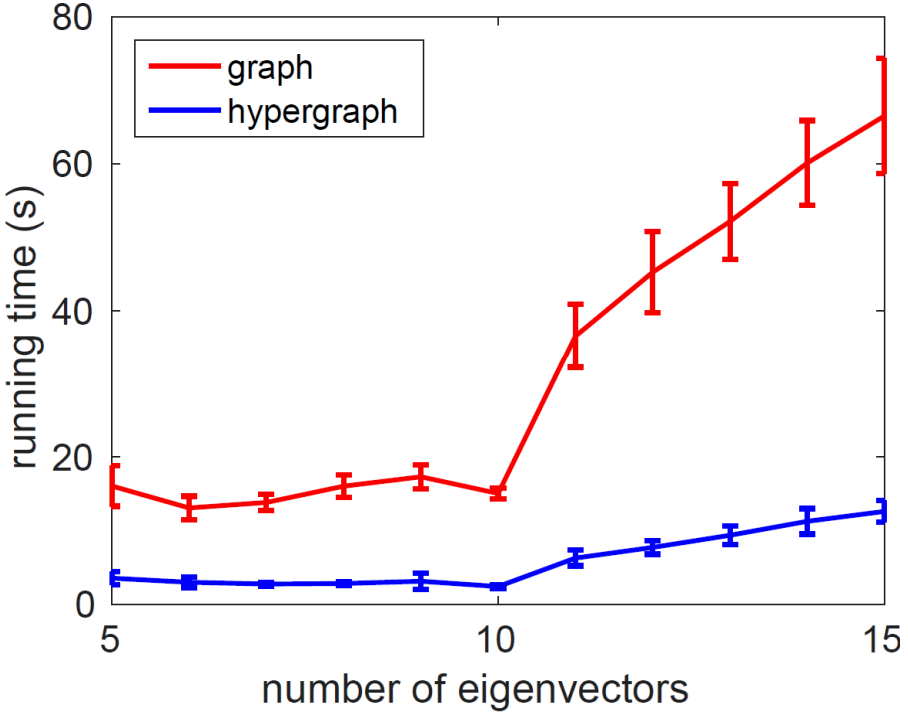
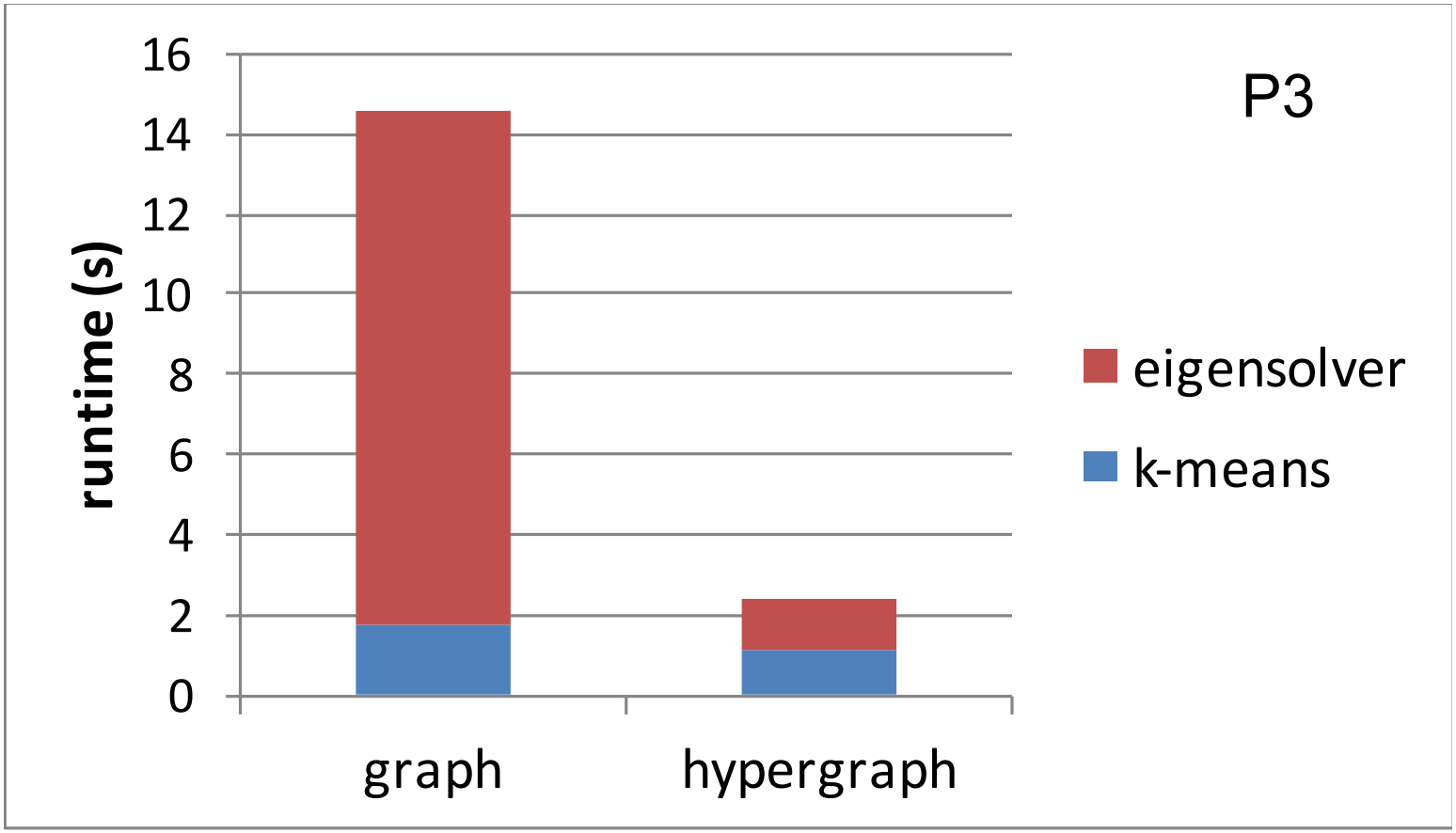




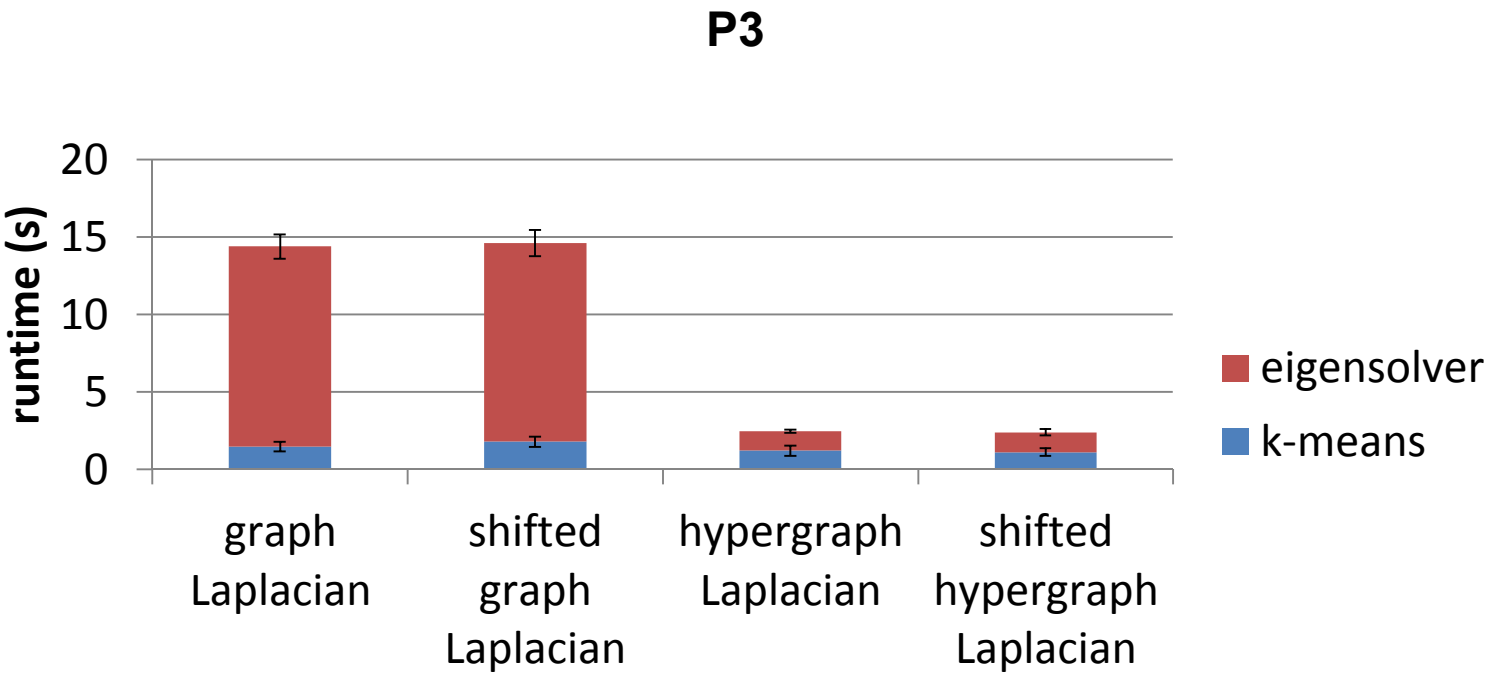
Noisier data: P3

Number of clusters	10
Nodes per cluster	10,000
Intra/Inter-cluster hyperedges	20,000 200,000
Intra/Inter-cluster h-edge cardinality	5 5

Runtimes: Eigensolver vs. K-means



Should we compute the eigenpairs of the Laplacian or the shifted Laplacian?



	Graph Laplacian L_g	Shifted graph Laplacian S_g	Hypergraph Laplacian L_h	Shifted hypergraph Laplacian S_h
LOBPCG iterations	15.6	15.6	8.9	8.9
K-means iterations	56.9	79.4	31.8	28.1

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Nodes per cluster	10,000
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Intra/Inter-cluster h-edge cardinality	5 5

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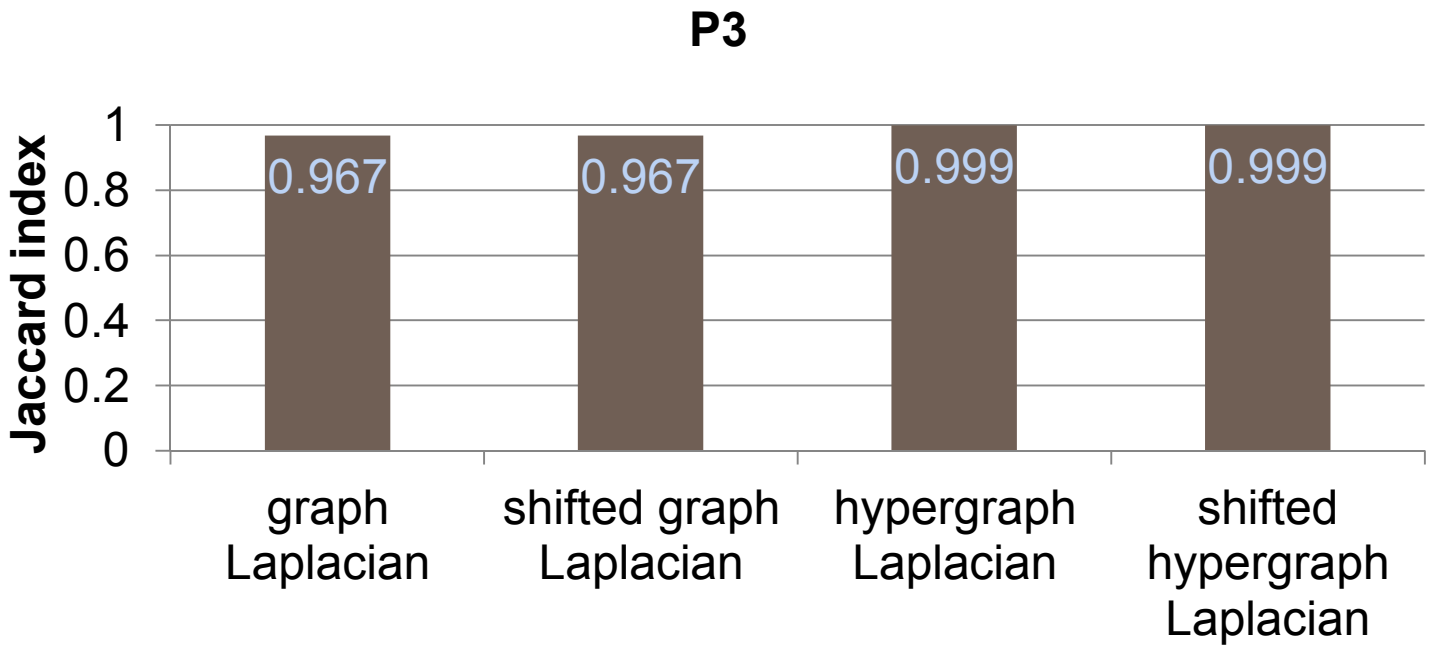

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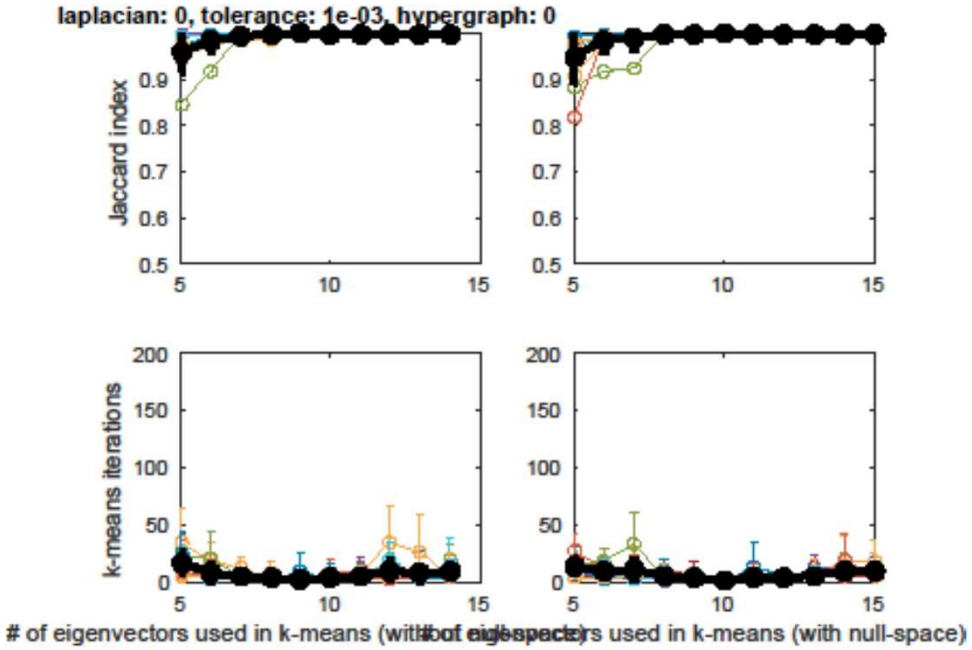
Number of clusters	10
Nodes per cluster	10,000
Intra/Inter-cluster hyperedges	20,000 200,000
Intra/Inter-cluster h-edge cardinality	5 5

Should the null space be provided to k-means?



- nClusters: 10
- nVerts: 10,000
- nEdges in cluster: 40,000
- nEdges between clusters: 50,000

Data Sets

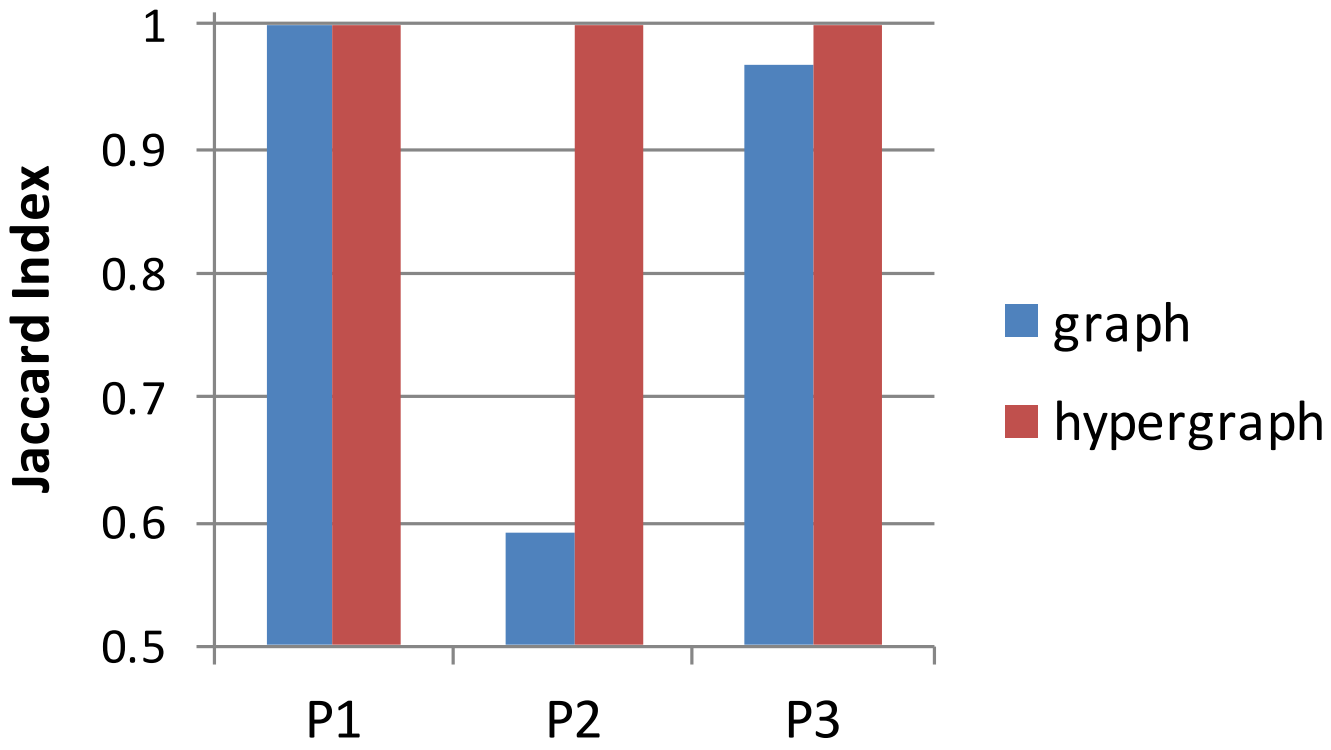
Sandia National Laboratories

	P1	P2	P3	Hyperedge Cardinality
Number of clusters	10	5	10	5
Vertices per cluster*	10,000	10,000	10,000	10,000
Intra-cluster hyperedges*	40,000	20,000	20,000	20,000
Inter-cluster hyperedges*	50,000	200,000	200,000	200,000
Intra-cluster hyperedge cardinality*	5	10	5	3-10
Inter-cluster hyperedge cardinality*	5	3	5	3-10

- Generate hypergraph incidence matrices
  - 4 different sets of parameters
  - Different levels of difficulties
  - 10 randomly generated hypergraphs for each parameter set

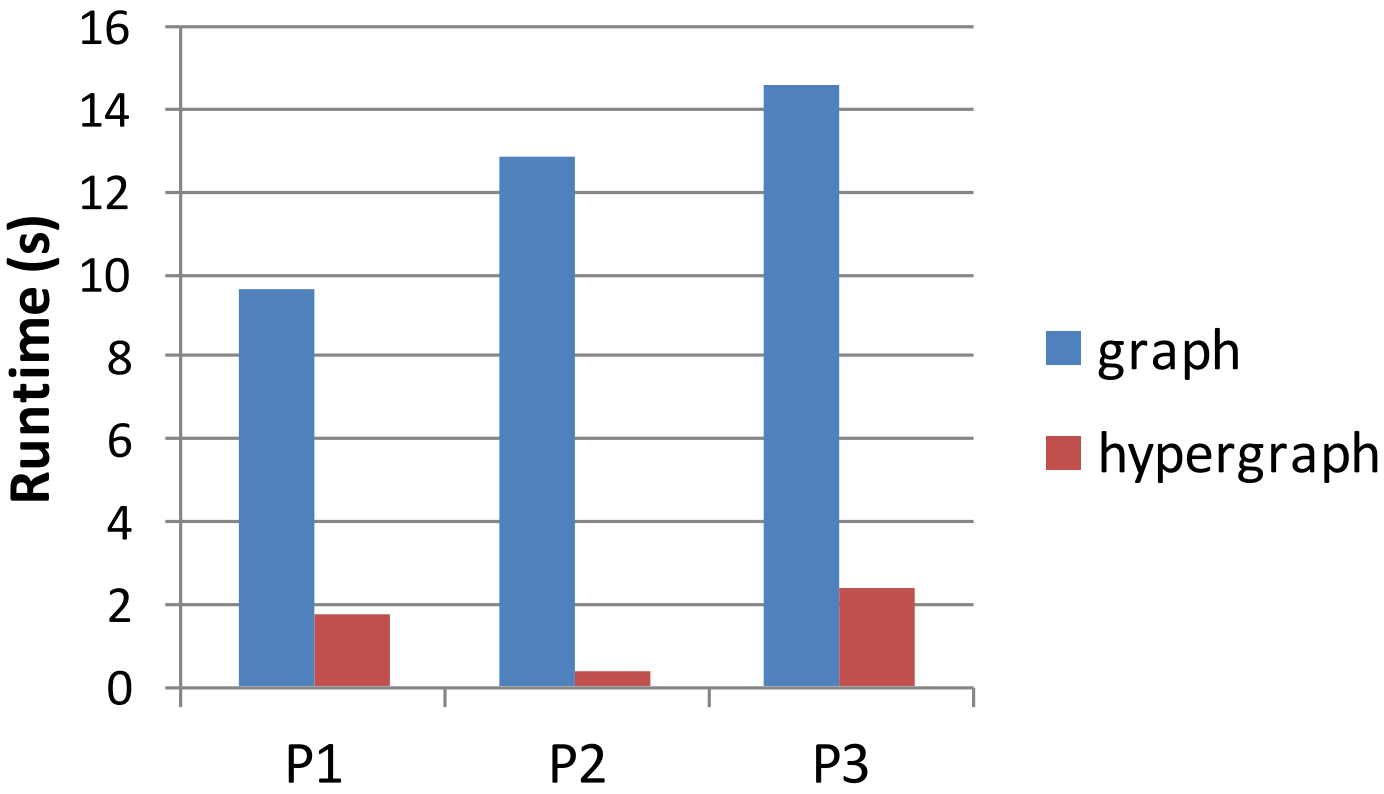
* Designates mean value

Clustering Quality: P1, P2, P3



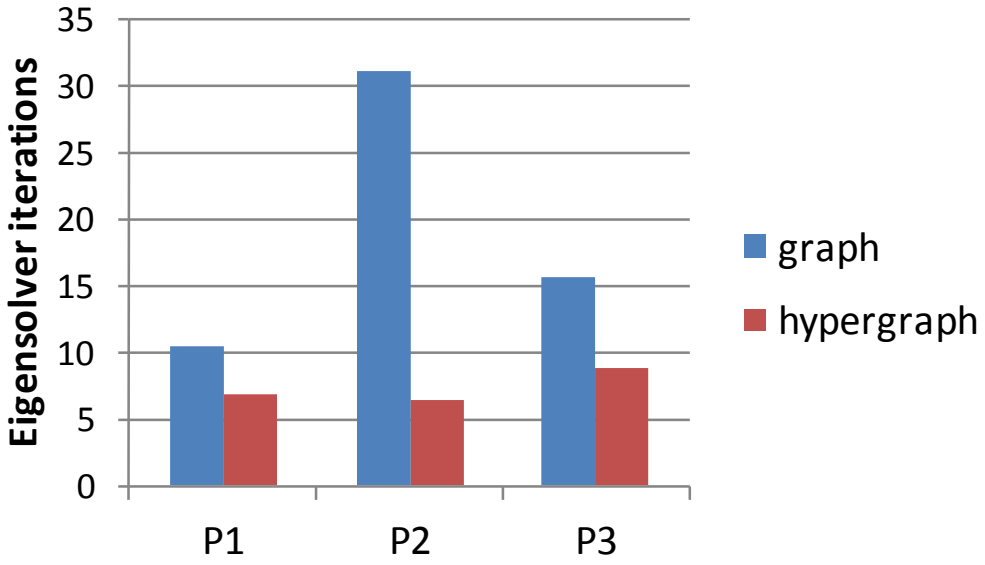
Hypergraph based clusters more similar to "ground truth" clusters than graph based clusters

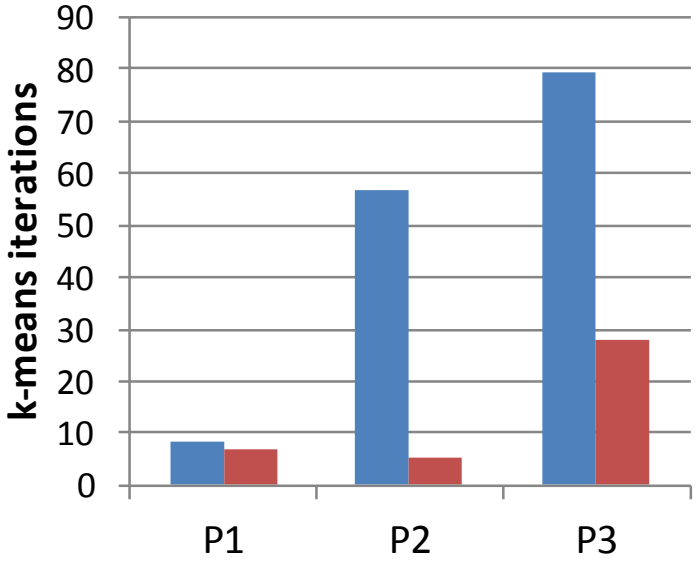
Runtimes: P1, P2, P3



Hypergraph models significantly more computationally efficient than graph models (up to 30x faster)

Iterations: P1, P2, P3

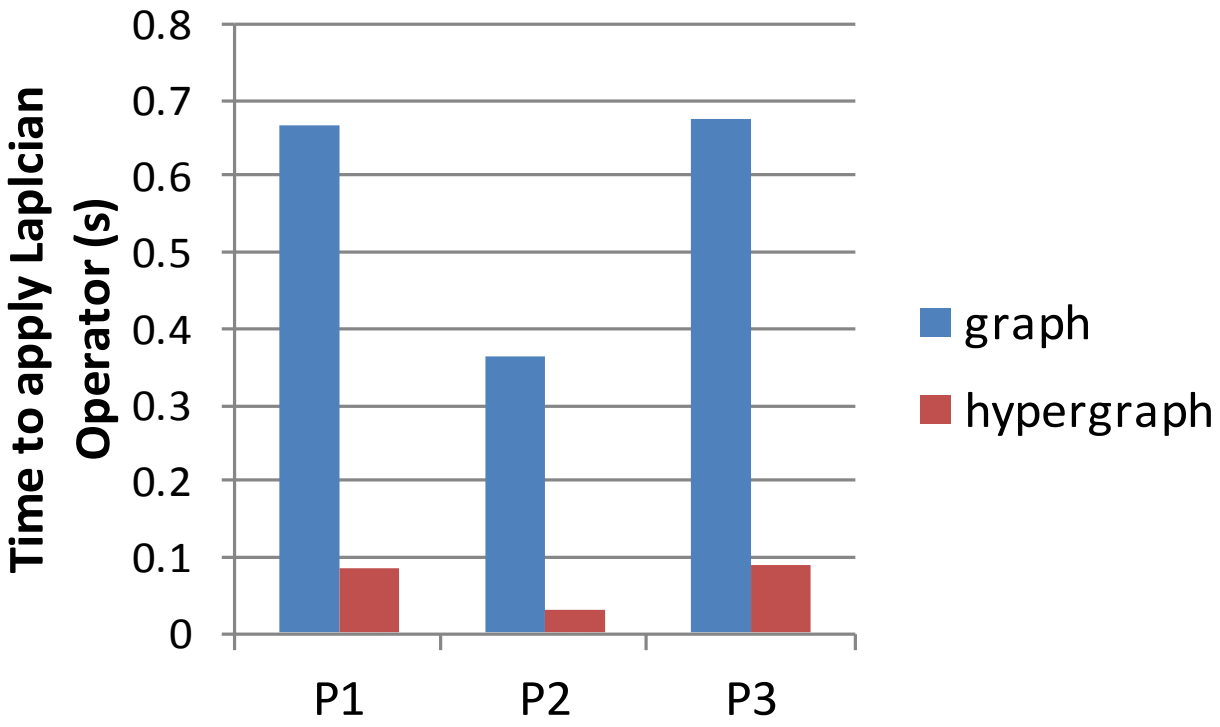




- Hypergraph required fewer LOBPCG iterations than graph
  - Better separation of eigenvalues in hypergraph Laplacian
- Hypergraph required fewer k-means iterations

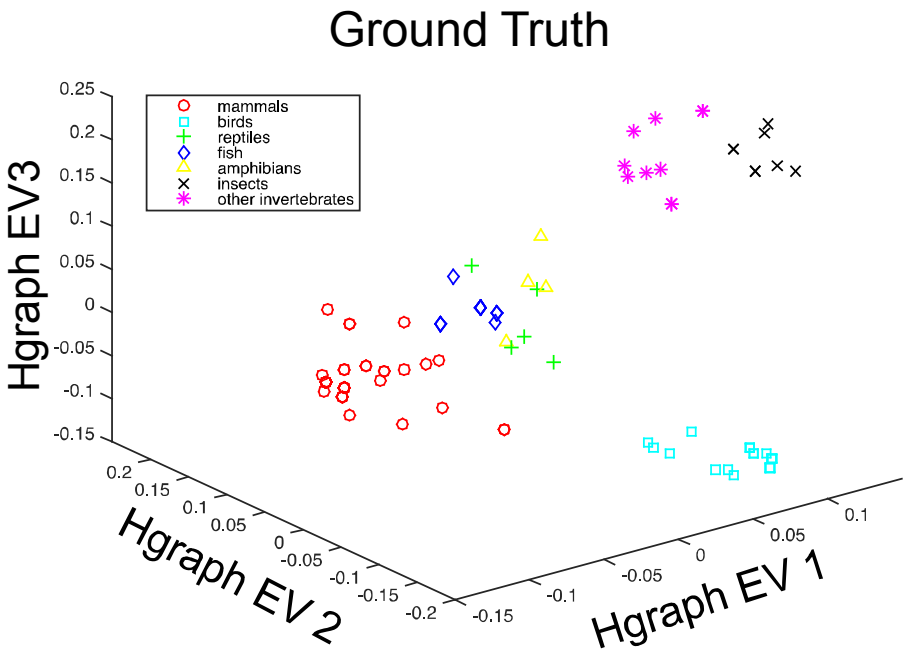
Hypergraph models converged faster than graph models

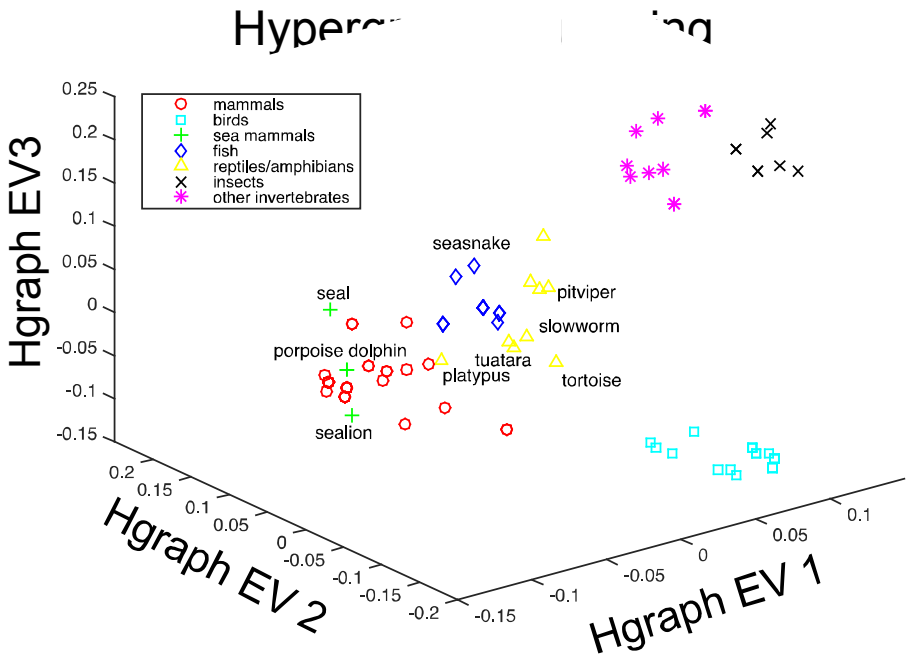
Laplacian Operator Apply: P1, P2, P3



Laplacian operator apply more efficient for hypergraph model than graph model (up to 12x faster)

Real Data – Hypergraph, 7 Clusters



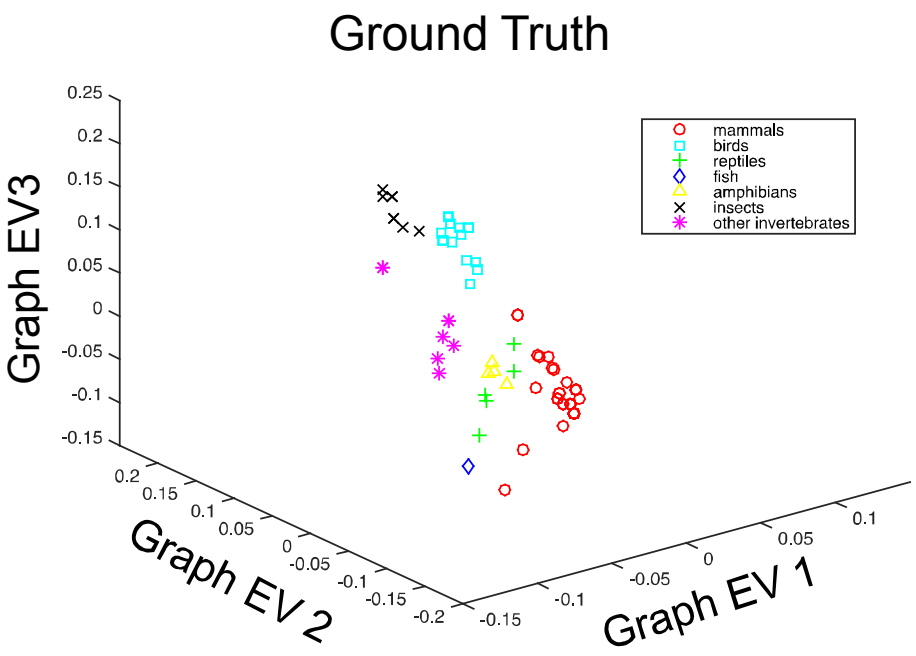


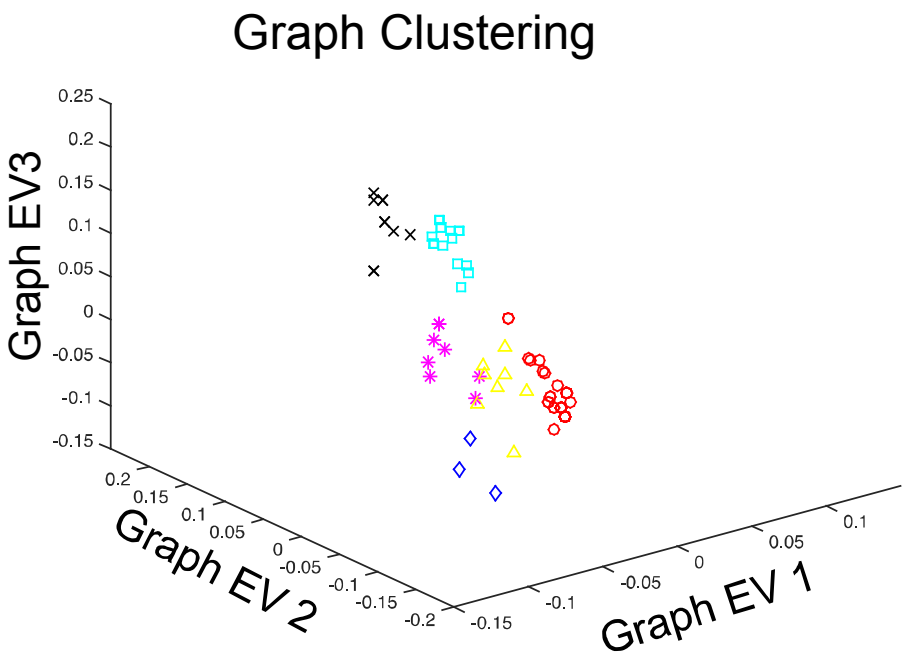
- UCI ML Repository Zoo Data Set*
  - Animals with 16 attributes (# legs, eggs, …) + category
- Hypergraph Clustering vs. ground truth for 7 clusters
  - Jaccard index: 0.815 (Graph model 0.743)
  - Merged reptiles/amphibians, new category: sea mammals

* https://archive.ics.uci.edu/ml/

EV=eigenvector

Real Data – Graph, 7 Clusters

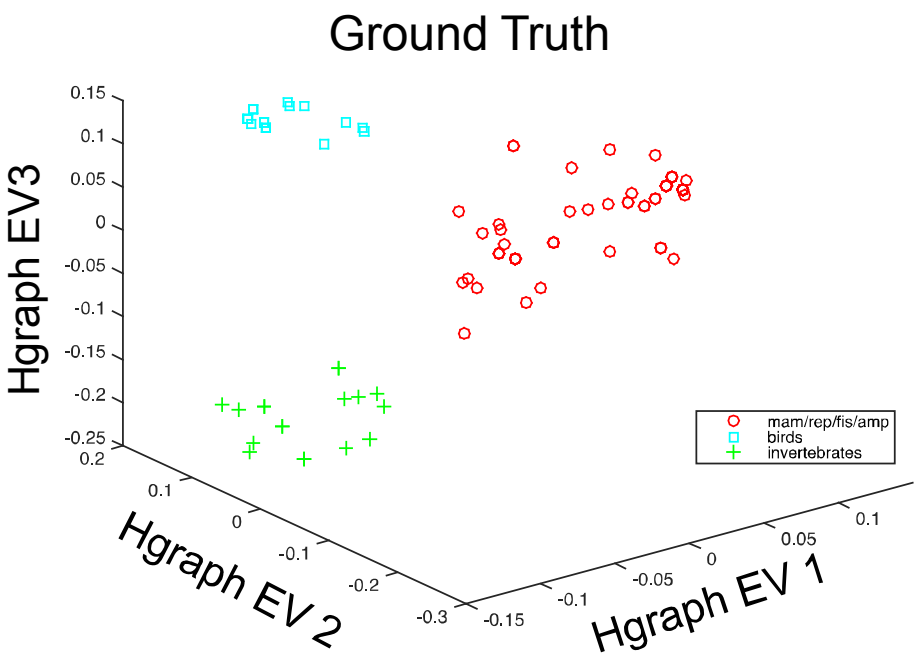


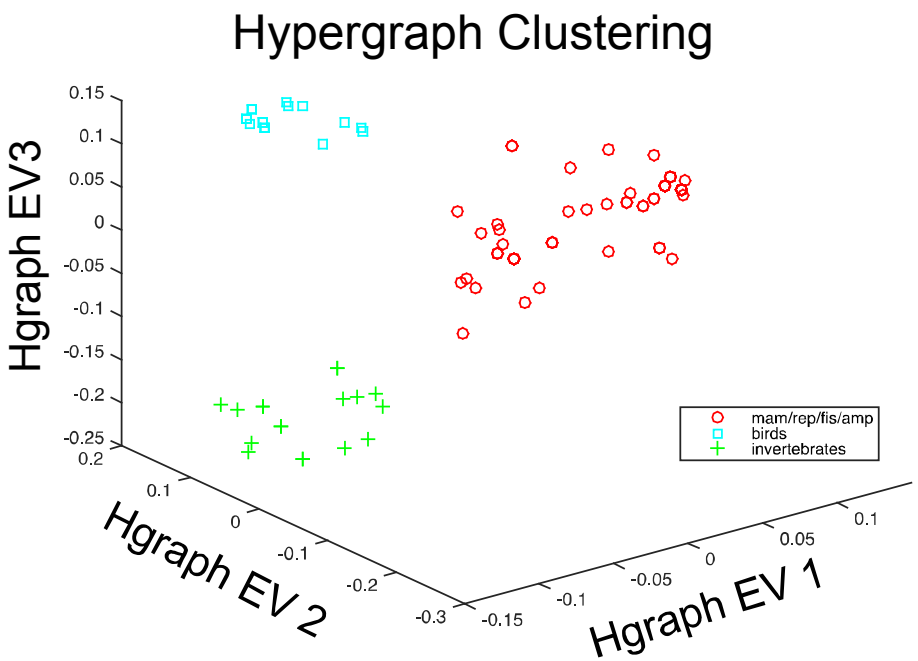


- Graph Clustering vs. ground truth for 7 clusters
  - Jaccard index: 0.743
  - Data harder for kmeans to separate
    - Insects, birds, mammals, other invertebrates, ?

EV=eigenvector

Real Data – Hypergraph, 3 Clusters



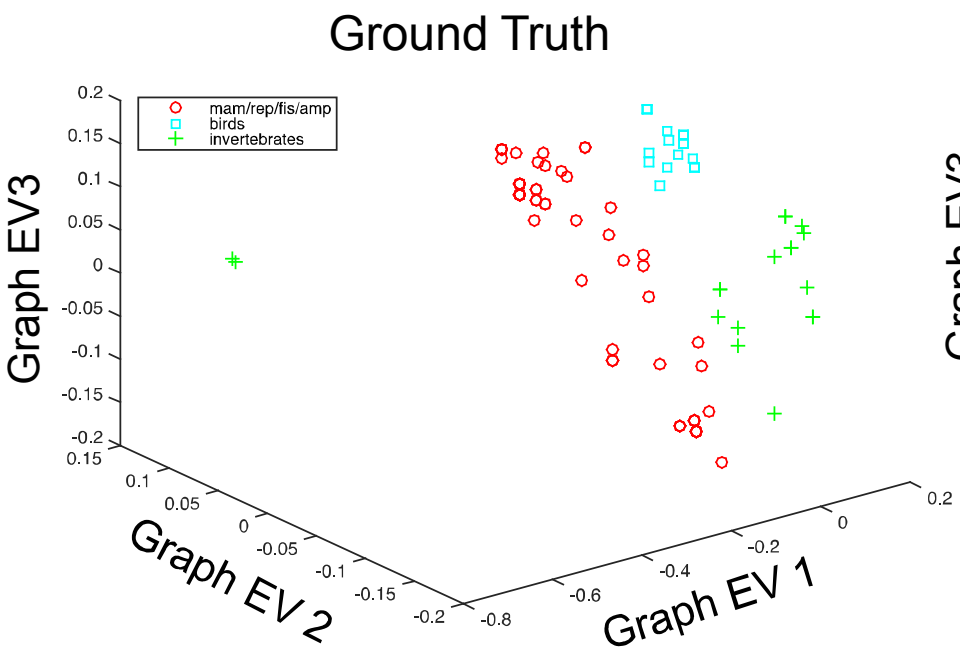


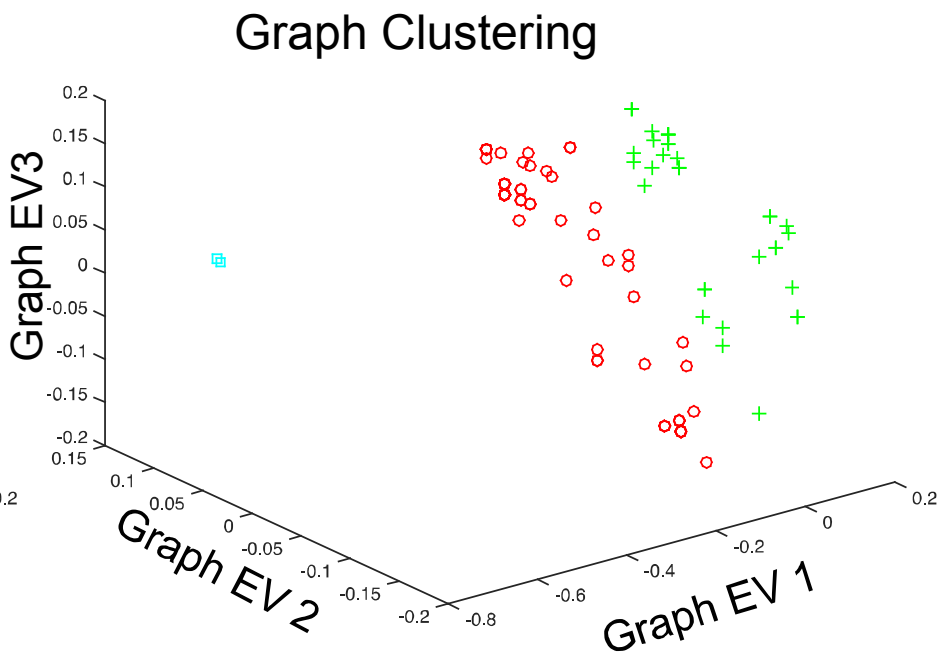
- UCI ML Repository Zoo Data Set*
  - Merged into 3 clusters: mammals/reptiles/fish/amphibians, birds, invertebrates
- Hypergraph Clustering vs. ground truth for 3 clusters
  - Jaccard index: 1.000 (Graph model 0.865)

* https://archive.ics.uci.edu/ml/

EV=eigenvector

Real Data – Graph, 3 Clusters





- Graph Clustering vs. ground truth for 3 clusters
  - Jaccard index: 0.865