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SAMSI - Aug 2010

(For more info, see: <u>http:// cs.stanford.edu/people/mmahoney/</u> or Google on "Michael Mahoney")

Lots of "networked data" out there!

- $\boldsymbol{\cdot}$ Technological and communication networks
 - AS, power-grid, road networks
- Biological and genetic networks
 - food-web, protein networks
- Social and information networks
 - collaboration networks, friendships; co-citation, blog crosspostings, advertiser-bidded phrase graphs ...
- Financial and economic networks
 - encoding purchase information, financial transactions, etc.
- Language networks
 - semantic networks ...
- Data-derived "similarity networks"
 - recently popular in, e.g., "manifold" learning
- ...

Sponsored ("paid") Search

Text-based ads driven by user query

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Sponsored Search Problems

Keyword-advertiser graph:

- provide new ads
- maximize CTR, RPS, advertiser ROI

Motivating cluster-related problems:

Marketplace depth broadening:

find new advertisers for a particular query/submarker

• Query recommender system:

suggest to advertisers new queries that have high probability of clicks

Contextual query broadening:

broaden the user's query using other context information



Micro-markets in sponsored search

Goal: Find *isolated* markets/clusters (in an advertiser-bidded phrase bipartite graph) with *sufficient money/clicks* with *sufficient coherence*.

Ques: Is this even possible?



How people think about networks

"Interaction graph" *model* of networks:

- Nodes represent "entities"
- Edges represent "interaction" between pairs of entities



Graphs are combinatorial, not obviously-geometric

- Strength: powerful framework for analyzing algorithmic complexity
- · Drawback: geometry used for learning and statistical inference

How people think about networks

A schematic illustration ...



Some evidence for micro-markets in sponsored search?



duery

advertiser

Questions of interest ...

What are degree distributions, clustering coefficients, diameters, etc.? Heavy-tailed, small-world, expander, geometry+rewiring, local-global decompositions, ... Are there natural clusters, communities, partitions, etc.? Concept-based clusters, link-based clusters, density-based clusters, ... (e.g., isolated micro-markets with sufficient money/clicks with sufficient coherence) How do networks grow, evolve, respond to perturbations, etc.? Preferential attachment, copying, HOT, shrinking diameters, ... How do dynamic processes - search, diffusion, etc. - behave on networks? Decentralized search, undirected diffusion, cascading epidemics, ... How best to do learning, e.g., classification, regression, ranking, etc.? Information retrieval, machine learning, ...

What do these networks "look" like?



Popular approaches to large network data



Heavy-tails and power laws (at *large size-scales*):

- extreme heterogeneity in local environments, e.g., as captured by degree distribution, and relatively unstructured otherwise
- basis for preferential attachment models, optimization-based models, power-law random graphs, etc.

Local clustering/structure (at *small size-scales*):

- local environments of nodes have structure, e.g., captures with clustering coefficient, that is meaningfully "geometric"
- basis for small world models that start with global "geometry" and add random edges to get small diameter and preserve local "geometry"



Popular approaches to data more generally



Use geometric data analysis tools:

- Low-rank methods very popular and flexible
- Manifold methods use other distances, e.g., diffusions or nearest neighbors, to find "curved" low-dimensional spaces

These geometric data analysis tools:

• View data as a point cloud in \mathbb{R}^n , i.e., each of the *m* data points is a vector in \mathbb{R}^n

- Based on SVD, a basic vector space structural result
- Geometry gives a lot -- scalability, robustness, capacity control, basis for inference, etc.



Can these approaches be combined?

These approaches are *very* different:

- network is a single data point---not a collection of feature vectors drawn from a distribution, and not really a matrix
- can't easily let m or n (number of data points or features) go to infinity---so nearly every such theorem fails to apply

Can associate matrix with a graph and vice versa, but:

- often do more damage than good
- questions asked tend to be very different
- graphs are really combinatorial things*

*But graph geodesic distance is a metric, and metric embeddings give fast algorithms!

Modeling data as matrices and graphs



In computer science:

• data are typically discrete, e.g., graphs

 focus is on fast algorithms for the given data set In statistics*:

- data are typically continuous, e.g.
 vectors
- focus is on inferring something about the world

*very broadly-defined!

What do the data "look like" (if you *squint* at them)?







(or pancake that embeds well in low dimensions)



(or tree-like hyperbolic structure)

A "point"?





(or clique-like or expander-like structure)





What is an expander?

Def: an *expander* is a "sparse" graph that does not have any "good" partitions into two or more pieces.

• E.g., a not-extremely-sparse random graph

Who cares?

• Expanders are metric spaces that are *least* like "low-dimensional" metric spaces

- Very important in TCS for algorithm design
- Large social and information are expanders ...

• (... at least more like pockets of local structure on global expanderlike scaffolding than vice versa, if you squint at them)



Popular algorithmic tools with a geometric flavor

Overview

• PCA, SVD; interpretations, kernel-based extensions; algorithmic and statistical issues; and limitations

Graph algorithms and their geometric underpinnings

• Spectral, flow, multi-resolution algorithms; their implicit geometric basis; global and scalable local methods; expander-like, tree-like, and hyperbolic structure

Novel insights on structure in large informatics graphs

• Successes and failures of existing models; empirical results, including "experimental" methodologies for probing network structure, taking into account algorithmic and statistical issues; implications and future directions



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The Singular Value Decomposition (SVD)

The formal definition:

Given any m x n matrix A, one can decompose it as:

$$\begin{pmatrix} A \\ \end{pmatrix} = \begin{pmatrix} U \\ W \end{pmatrix} \cdot \begin{pmatrix} \Sigma \\ P \times \rho \end{pmatrix} \cdot \begin{pmatrix} V \end{pmatrix}^{T}$$

$$m \times \rho \quad \rho \times \rho \quad \rho \times n$$

- $\rho : \textbf{rank of A}$
- U (V): orthogonal matrix containing the left (right) singular vectors of A.
- Σ : diagonal matrix containing $\sigma_1 \ge \sigma_2 \ge ... \ge \sigma_{\rho}$, the singular values of A.

SVD is the "the Rolls-Royce and the Swiss Army Knife of Numerical Linear Algebra."* *Dianne O'Leary, MMDS 2006



 $U_k(V_k)$: orthogonal matrix containing the top k left (right) singular vectors of A. Σ_k : diagonal matrix containing the top k singular values of A.

<u>Important</u>: Keeping top k singular vectors provides "best" rank-k approximation to A (w.r.t. Frobenius norm, spectral norm, etc.):

 $A_k = \operatorname{argmin}\{ ||A-X||_{2,F} : \operatorname{rank}(X) \le k \}.$

Singular values, intuition



Blue circles are *m* data points in a 2-D space.

The SVD of the *m-by-2* matrix of the data will return ...

V⁽¹⁾: <u>1st (right) singular vector</u>: direction of maximal variance,

 σ_1 : how much of data variance is explained by the first singular vector.

V⁽²⁾: <u>2nd (right) singular vector</u>: direction of maximal variance, after removing projection of the data along first singular vector.

 σ_2 : measures how much of the data variance is explained by the second singular vector.



• Sometimes people interpret document corpus in terms of k topics when use this.

• Better to think of this as just selecting one model from a parameterized class of models!

LSI/SVD and heavy-tailed data

Theorem: (Mihail and Papadimitriou, 2002)

The largest eigenvalues of the adjacency matrix of a graph with power-law distributed degrees are also power-law distributed.

• I.e., heterogeneity (e.g., heavy-tails over degrees) plus noise (e.g., random graph) implies heavy tail over eigenvalues.

• Intuitive Idea: 10 components may give 10% of mass/information, but to get 20%, you need 100, and to get 30% you need 1000, etc; i.e., no scale at which you get most of the information

• No "latent" semantics without preprocessing.



Mahoney and Drineas (PNAS, 2009)



Reification

 assigning a "physical reality" to large singular directions

invalid in general

Just because "If the data are 'nice' then SVD is appropriate" does NOT imply converse.



Interpretation: Centrality

Centrality (of a vertex) - measures relative importance of a vertices in a graph

- degree centrality number of links incident upon a node
- betweenness centrality high for vertices that occur on many shortest paths
- closeness centrality mean geodesic distance between a vertex and other reachable nodes

• eigenvector centrality - connections to high-degree nodes are more important, and so on iteratively (a "spectral ranking" measure)

Motivation and behavior on nice graphs is clear -- but what do they actually compute on non-nice graphs?

Eigen-methods in ML and data analysis

Eigen-tools appear (*explicitly* or *implicitly*) in many data analysis and machine learning tools:

- Latent semantic indexing
- PCA and MDS
- Manifold-based ML methods
- Diffusion-based methods
- k-means clustering
- Spectral partitioning and spectral ranking



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Graph partitioning

- A family of combinatorial optimization problems want to partition a graph's nodes into two sets s.t.:
- Not much edge weight across the cut (cut quality)
- Both sides contain a lot of nodes

Several standard formulations:

- Graph bisection (minimum cut with 50-50 balance)
- + β -balanced bisection (minimum cut with 70-30 balance)
- cutsize/min{|A|,|B|}, or cutsize/(|A||B|) (expansion)
- cutsize/min{Vol(A),Vol(B)}, or cutsize/(Vol(A)Vol(B)) (conducta)



All of these formalizations of the bi-criterion are NP-hard!

Why worry about both criteria?

• Some graphs (e.g., "space-like" graphs, finite element meshes, road networks, random geometric graphs) cut quality and cut balance "work together"

Tradeoff between cut quality and balance



• For still other graphs (e.g., expanders) there are no good cuts of any size

Why graph partitioning?

Graph partitioning algorithms:

- · capture a qualitative notion of connectedness
- well-studied problem in traditionally/recently both in theory and practice
- many machine learning and data analysis applications

Don't care about exact solution to intractable problem:

- output of approximation algs is not something we "settle for"
 randomized/approximation algs often give "better" answers than exact solution
- nearly-linear/poly-time computation captures "qualitative existence"

The "lay of the land"

Spectral methods* - compute eigenvectors of associated matrices

Local improvement - easily get trapped in local minima, but can be used to clean up other cuts

Multi-resolution - view (typically space-like graphs) at multiple size scales

Flow-based methods* - single-commodity or multicommodity version of max-flow-min-cut ideas

*comes with strong worst-case guarantees

Spectral Methods

Fiedler (1973) and Donath & Hoffman (1973)

• use eigenvectors of discrete graph Laplacian

Popular in scientific computing, parallel computing, etc. (1980s) and machine learning (2000s)

Algorithm:

1. Compute the exact/approximate eigenvector.

2. Perform "rounding": choose the best of the n cuts defined by that eigenvector.

An "embedding" view of spectral

Use Rayleigh quotient to characterize λ_1 :

$$\lambda_1 = \min_{x \perp D1} \frac{\sum_{i \sim j} (x_i - x_j)^2}{\sum_i x_i^2 d_i}$$

Interpretation:

- Minimize "mixing" subject to variance constraint
- Embed graph on a line and cut
- But duality not tight

But since $x \perp D1$, this is equivalent to:

$$\frac{\lambda_1}{\operatorname{vol}(G)} = \min_{x \perp D1} \frac{\sum_{i \sim j} (x_i - x_j)^2}{\sum_{i,j} (x_i - x_j)^2 d_i d_j}$$

Interpretation:

- Minimize "mixing" subject to "mixing" in complete graph K_n
- Embed graph in (scaled) K_n
- Duality tighter (can also see this in dual later)

Maximum flow problem

- Directed graph G=(V,E).
- Source s ϵ V, sink t ϵ V.
- Capacity c(e) ϵ Z⁺ for each edge e.
- Flow: function f: E -> N s.t.
- For all e: f(e) ≤ c(e)
- For all v, except s and t: flow into v = flow out of v
- Flow value: flow out of s
- Problem: find flow from s to t with maximum value

Important Variant: Multiple Sources and Multiple Sinks



An "embedding" view of flow

Theorem: (Bourgain)

Every n-point metric space embeds into L1 with distortion O (log(n)).

Flow-based algorithm to get sparsest cuts.

- (1) Solve LP to get distance d:V×V->R+.
- (2) Obtain L1 embedding using Bourgain's constructive theorem
- (3) Perform an appropriate "rounding."

Thus, it boils down to an embedding and expanders are worst.
"Spectral" versus "flow"

Spectral:

- Compute an eigenvector
- "Quadratic" worst-case bounds
- Worst-case achieved -- on "long stringy" graphs
- Embeds you on a line (or complete graph)

Flow:

- Compute a LP
- O(log n) worst-case bounds
- Worst-case achieved -- on expanders
- Embeds you in L1

Two methods -- complementary strengths and weaknesses

• What we compute will be determined at least as much by as the approximation algorithm we use as by objective function.

Extensions of the basic ideas

Cut improvement algorithms

• Given an input cut, find a good one nearby or certify that none exists

Local algorithms and locally-biased objectives

• Run in a time depending on the size of the output and/or are biased toward input seed set of nodes

Combining spectral and flow

• to take advantage of their complementary strengths

Interplay between preexisting versus generated versus implicit geometry

Preexisting geometry

Start with geometry and add "stuff"

Generated geometry

• Generative model leads to structures that are meaningfully-interpretable as geometric

Implicitly-imposed geometry

• Approximation algorithms implicitly embed the data in a metric/geometric place and then round.







What is the *shape* of a graph?

Can we generalize the following intuition to general graphs:

- A 2D grid or well-shaped mesh "looks like" a 2D plane
- A random geometric graph "looks like" a 2D plane
- An expander "looks like" a clique or complete graph or a point.

The basic idea:

• If a graph embeds well in another metric space, then it "looks like" that metric space**!

**Gromov (1987); Linial, London, & Rabinovich (1985); ISOMAP, LLE, LE, ... (2001)

Hyperbolic Spaces

Lobachevsky and Bolyai constructed ^{c1} hyperbolic space - (between a point and a line, there are many "parallel" lines) - Euclid's fifth postulate is independent of the others!

A d-dimensional metric space which is homogeneous and isotropic (looks the same at every point and in every direction) is locally identical to one of:

- Sphere
- Hyperbolic space
- Euclidean plane

The 3 maximally symmetric geometries

A1



В

D1

B1 D

Comparison between different curvatures

Property	Euclid.	Spherical	Hyperbolic
Curvature	0	1	-1
Parallel lines	1	0	∞
Triangles are	normal	thick	thin
Shape of trian- gles	\triangle	\bigcirc	$ \land $
Sum of angles	π	$> \pi$	$<\pi$
Circle length	$2\pi R$	$2\pi \sin R$	$2\pi \sinh R$
Disc area	$2\pi R^{2}/2$	$2\pi(1-\cos R)$	$2\pi(\cosh R - 1)$

δ -hyperbolic metric spaces

Definition: [Gromov, 1987] A graph is δ -hyperbolic iff: For every 4 vertices u, v, w, and z, the larger 2 of the 3 distance sums, d(u, v) + d(w, z) and d(u, w) + d(v, z) and d(u, z) + d(v, w), differ by at most 2δ .

Things to note about δ -hyperbolicity:

• Graph property that is both *local* (by four points) and *global* (by the distance) in the graph

- Polynomial time computable naively in $O(n^4)$ time
- Metric space embeds into a tree iff δ = 0.
- Poincare half space in R^k is δ -hyperbolic with δ = log_23
- Theory of δ -hyperbolic spaces generalize theory of Riemannian manifold with negative sectional curvature to metric spaces

Expanders and hyperbolicity

Different concepts that really are different (Benjamini 1998):

- Constant-degree expanders like sparsified complete graphs
- Hyperbolic metric space like a tree-like graph

But, *degree heterogeneity enhances hyperbolicity** (so real networks will often have both properties).

*Question: Does anyone know a reference that makes these connections precise?

Trees come in all sizes and shapes:





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An awkward empirical fact

Lang (NIPS 2006), Leskovec, Lang, Dasgupta, and Mahoney (WWW 2008 & arXiv 2008)

Can we cut "internet graphs" into two pieces that are "nice" and "well-balanced?



For many **real-world** social-and-information "power-law graphs," there is an *inverse* relationship between "cut quality" and "cut balance."

Consequences of this empirical fact

Relationship b/w small-scale structure and largescale structure in social/information networks* is not reproduced (even qualitatively) by popular models

- This relationship governs diffusion of information, routing and decentralized search, dynamic properties, etc., etc., etc.
- This relationship also governs (implicitly) the applicability of nearly every common data analysis tool in these apps

*Probably *much* more generally--social/information networks are just so messy and counterintuitive that they provide very good methodological test cases.

Popular approaches to network analysis



Define simple statistics (clustering coefficient, degree distribution, etc.) and fit simple models

- more complex statistics are too algorithmically complex or statistically rich
- fitting simple stats often doesn't capture what you wanted

Beyond very simple statistics:

• Density, diameter, routing, clustering, communities, ...



• Popular models often fail egregiously at reproducing more subtle properties (even when fit to simple statistics)

Failings of "traditional" network approaches

- Three recent examples of *failings* of "small world" and "heavy tailed" approaches:
- Algorithmic decentralized search solving a (non-ML) problem: can we find short paths?
- Diameter and density versus time simple dynamic property
- Clustering and community structure subtle/complex static property (used in downstream analysis)

All three examples have to do with the **coupling b/w** "local" structure and "global" structure --- solution goes beyond simple statistics of traditional approaches.

Failing 1: Search in social graphs

Milgram (1960s)



- Small world experiments study short paths in social networks
- Individuals from Midwest forward letter to people they know to get it to an individual in Boston.

Watts and Strogatz (1998)



- "Small world" model, i.e., add random edges to an underlying local geometry, reproduces local clustering and existence of short paths *Kleinberg (2000)*
- But, even Erdos-Renyi G_{np} random graphs have short paths ...
- ... so the existence of short paths is not so interesting
- Milgram's experiment also demonstrated people found those paths

Failing 2: Time evolving graphs

Albert and Barabasi (1999)



- "Preferential attachment" model, i.e., at each time step add a constant number of links according to a "rich-get-richer" rule
- Constant average degree, i.e., average node degree remains constant
- Diameter increases roughly logarithmically in time

Leskovec, Kleinberg, and Faloutsos (2005)

• But, *empirically*, graphs densify over time (i.e., number of edges grows superlinearly with number of nodes) and diameter shrinks over time

Failing 3: Clustering and community structure

Sociologists (1900s)

• A "community" is any group of two or more people that is useful Girvan and Newman (2002,2004) and MANY others



• A "community" is a set of nodes "joined together in tightly-knit groups between which there are only loose connections

• Modularity becomes a popular "edge counting" metric

Leskovec, Lang, Dasgupta, and Mahoney (2008)



• All work on community detection validated on networks with good well-balanced partitions (i.e., low-dimensional and not expanders)

• But, *empirically*, larger clusters/communities are less-and-less cluster-like than smaller clusters (i.e., networks are expander-like)

What do these networks "look" like?



Exptl Tools: Probing Large Networks with Approximation Algorithms

Idea: Use approximation algorithms for NP-hard graph partitioning problems as experimental probes of network structure.

Spectral - (quadratic approx) - confuses "long paths" with "deep cuts" Multi-commodity flow - (log(n) approx) - difficulty with expanders

SDP - (sqrt(log(n)) approx) - best in theory

Metis - (multi-resolution for mesh-like graphs) - common in practice

X+MQI - post-processing step on, e.g., Spectral of Metis

Metis+MQI - best conductance (empirically)

Local Spectral - connected and tighter sets (empirically, regularized communities!)

We are not interested in partitions per se, but in probing network structure.

Analogy: What does a protein look like?



Three possible representations (all-atom; backbone; and solvent-accessible surface) of the three-dimensional structure of the protein triose phosphate isomerase.

background medium



Experimental Procedure:

- Generate a bunch of output data by using the unseen object to filter a known input signal.
- Reconstruct the unseen object given the output signal and what we know about the artifactual properties of the input signal.

Communities, Conductance, and NCPPs

Let A be the adjacency matrix of G=(V,E). The conductance ϕ of a set S of nodes is:

$$\phi(S) = \frac{\sum_{i \in S, j \notin S} A_{ij}}{\min\{A(S), A(\overline{S})\}}$$

$$A(S) = \sum_{i \in S} \sum_{j \in V} A_{ij}$$

The Network Community Profile (NCP) Plot of the graph is:

$$\Phi(k) = \min_{S \subset V, |S|=k} \phi(S)$$

Since algorithms often have non-obvious sizedependent behavior.

Just as conductance captures the "gestalt" notion of cluster/community quality, the NCP plot measures cluster/community quality as a function of size. NCP is intractable to compute --> use approximation algorithms!

Community Score: Conductance

- How community like is a set of nodes?
- Need a natural intuitive measure:



Conquerance (normanzea cur)

 ϕ (S) \approx # edges cut / # edges inside

 Small (S) corresponds to more community-like sets of nodes













Widely-studied small social networks





Newman's Network Science

"Low-dimensional" graphs (and expanders)



NCPP for common generative models 10⁰ 10⁰ φ (conductance) ϕ (conductance) 10⁻¹ 10⁻¹ **Original network** Original network Rewired network Rewired network 10⁻² 10⁻² 10^{3} 10^{0} 10^{2} 10^{4} 10^{2} 10^{3} 10^{1} 10⁰ 10^{1} n (number of nodes in the cluster) n (number of nodes in the cluster) **Preferential Attachment** Copying Model 10⁰ 10⁰ φ (conductance) φ (conductance) 10⁻¹ 10⁻¹ Original network Original network Rewired network **Rewired network** 10⁻² 10⁻² TITU 10⁰ 10⁰ 10^{3} 10^{3} 10^{2} 10^{4} 10⁵ 10^{2} 10⁴ 10^{1} 10^{1} n (number of nodes in the cluster) n (number of nodes in the cluster) **Geometric PA RB** Hierarchical

What do large networks look like?

Downward sloping NCPP

small social networks (validation)

"low-dimensional" networks (intuition)

hierarchical networks (model building)

existing generative models (incl. community models)

Natural interpretation in terms of isoperimetry

implicit in modeling with low-dimensional spaces, manifolds, k-means, etc.

Large social/information networks are very very different

We examined more than 70 large social and information networks We developed principled methods to interrogate large networks Previous community work: on small social networks (hundreds, thousands)

Large Social and Information Networks

• Social nets	Nodes	Edges	Description	
LIVEJOURNAL	4,843,953	42,845,684	Blog friendships [4]	
Epinions	75,877	405,739	Who-trusts-whom [35]	
FLICKR	404,733	2,110,078	Photo sharing [21]	
Delicious	147,567	301,921	Collaborative tagging	
CA-DBLP	317,080	1,049,866	Co-authorship (CA) [4]	
CA-COND-MAT	21,363	91,286	CA cond-mat [25]	
• Information networks				
Cit-hep-th	27,400	352,021	hep-th citations [13]	
Blog-Posts	437,305	565,072	Blog post links [28]	
• Web graphs				
Web-google	855,802	4,291,352	Web graph Google	
Web-wt10g	1,458,316	6,225,033	TREC WT10G web	
• Bipartite affiliation (authors-to-papers) networks				
ATP-DBLP	615,678	944,456	DBLP [25]	
ATP-ASTRO-PH	54,498	131,123	Arxiv astro-ph [25]	
• Internet networks				
AS	6,474	12,572	Autonomous systems	
GNUTELLA	62,561	147,878	P2P network [36]	

Table 1: Some of the network datasets we studied.





Focus on the red curves (local spectral algorithm) - blue (Metis+Flow), green (Bag of whiskers), and black (randomly rewired network) for consistency and cross-validation.

More large networks 10⁰ 10⁰ ϕ (conductance) 10^{-1} ϕ (conductance) 10⁻¹ 10⁻² 10⁻³ 10⁻² 10⁻⁴ 10⁵ 10⁰ 10² 10^{3} 10⁴ 10⁵ 10⁰ 10^{2} 10³ 10⁴ 10⁶ 10^{1} 10^{1} n (number of nodes in the cluster) n (number of nodes in the cluster) Cit-Hep-Th Web-Google 10⁰ 10⁰ ϕ (conductance) ϕ (conductance) 10⁻¹ 10⁻¹ 10⁻² 10⁻² 10⁻³ 10⁴ 10⁰ 10² 10³ 10⁵ 10⁶ 10⁰ 10² 10³ 10⁵ 10^{4} 10^{1} 10^{1} n (number of nodes in the cluster) n (number of nodes in the cluster) Gnutella AtP-DBLP

NCPP: LiveJournal (N=5M, E=43M)



How do we know this plot it "correct"?

- Algorithmic Result
 - Ensemble of sets returned by different algorithms are very different Spectral vs. flow vs. bag-of-whiskers heuristic
- Statistical Result

Spectral method implicitly regularizes, gets more meaningful communities

Lower Bound Result

Spectral and SDP lower bounds for large partitions

Structural Result

Small barely-connected "whiskers" responsible for minimum

Modeling Result

Very sparse Erdos-Renyi (or PLRG wth $\beta \epsilon$ (2,3)) gets imbalanced deep cuts

Other clustering methods

- LeightonRao: based on multi-commodity flow
 - Disconnected clusters vs.
 Connected clusters
- Graclus prefers larger clusters
- Newman's modularity optimization similar to Local Spectral


12 objective functions

Clustering objectives:

- Single-criterion:
 - Modularity: *m*-*E*(*m*) (Volume minus correction)
 - Modularity Ratio: *m*-*E*(*m*)
 - Volume: $\sum_{u} d(u) = 2m + c$
 - Edges cut: *c*
- Multi-criterion:
 - <u>Conductance</u>: c/(2m+c) (SA to Volume)
 - Expansion: *c*/*n*
 - Density: $1 m/n^2$
 - CutRatio: c/n(N-n)
 - Normalized Cut: c/(2m+c) + c/2(M-m)+c
 - Max ODF: max frac. of edges of a node pointing outside S
 - Average-ODF: avg. frac. of edges of a node pointing outside
 - Flake-ODF: frac. of nodes with mode than ¹/₂ edges inside

S

n: nodes in Sm: edges in Sc: edges pointing outside S

Multi-criterion objectives



- Qualitatively similar to conductance
- Observations:
 - Conductance, Expansion, NCut, Cutratio and Avg-ODF are similar
 - Max-ODF prefers smaller clusters
 - Flake-ODF prefers larger clusters
 - Internal density is bad
 - Cut-ratio has high variance

Avg ODF

Flake ODF

Single-criterion objectives



Observations:

- All measures are monotonic (for rather trivial reasons)
- Modularity
 - prefers large clusters
 - Ignores small clusters
 - Because it basically captures Volume!

Volume

Edges cut

Lower and upper bounds

- Lower bounds on conductance can be computed from:
 - Spectral embedding (independent of balance)
 - SDP-based methods (for volume-balanced partitions)
- Algorithms find clusters close to theoretical lower bounds





φ (conductance)



"Whiskers" and the "core"

- "Whiskers"
 - maximal sub-graph detached from network by removing a single edge
 - contains 40% of nodes and 20% of edges
- "Core"
 - the rest of the graph, i.e., the 2-edge-connected core
- Global minimum of NCPP is a whisker
- BUT, core itself has nested whiskercore structure



What if the "whiskers" are removed?

Then the lowest conductance sets - the "best" communities - are "2-whiskers." (So, the "core" peels apart like an onion.)





Small versus Large Networks

Leskovec, et al. (arXiv 2009); Mahdian-Xu 2007

Small and large networks are very different:

(also, an expander)



Will be well
Will be well<

E.g., fit these networks to Stochastic Kronecker Graph with "base" K=[a b; b c]:

K_1 =	0.99	0.17		0.99	0.55
	0.17	0.82		0.55	0.15

0.2	0.2
0.2	0.2



Small versus Large Networks

Leskovec, et al. (arXiv 2009); Mahdian-Xu 2007

Small and large networks are very different:

(also, an expander)





E.g., fit these networks to Stochastic Kronecker Graph with "base" K=[a b; b c]:







Interpretation: A simple theorem on random graphs

Let $\mathbf{w} = (w_1, \dots, w_n)$, where $w_i = ci^{-1/(\beta-1)}, \quad \beta \in (2,3).$ Connect nodes *i* and *j* w.p. $p_{ij} = w_i w_j / \sum_k w_k.$





Structure of the G(w) model, with $\beta \epsilon$ (2,3).

- Sparsity (coupled with randomness) is the issue, not heavy-tails.
- (Power laws with $\beta \ \epsilon$ (2,3) give us the appropriate sparsity.)

Regularized and non-regularized communities (1 of 2)



- Metis+MQI (red) gives sets with better conductance.
- Local Spectral (blue) gives tighter and more well-rounded sets.



Regularized and non-regularized communities (2 of 2)

Two ca. 500 node communities from Local Spectral Algorithm:



Two ca. 500 node communities from Metis+MQI:





Implications: high level

What is simplest explanation for empirical facts?

• *Extremely* sparse Erdos-Renyi reproduces qualitative NCP (i.e., deep cuts at small size scales and no deep cuts at large size scales) since:

sparsity + randomness = measure fails to concentrate

• Power law random graphs also reproduces qualitative NCP for analogous reason

• Iterative forest-fire model gives mechanism to put local geometry on sparse quasi-random scaffolding to get qualitative property of relatively gradual increase of NCP

Data are local-structure on global-noise, not small noise on global structure!

Degree heterogeneity and hyperbolicity

Social and information networks are expander-like at large size scales, but:

• Degree heterogeneity enhances hyperbolicity

Lots of evidence:

• Scale free and internet graphs are more hyperbolic than other models, MC simulation -Jonckheere and Lohsoonthorne (2007)

• Mapping network nodes to spaces of negative curvature leads to scale-free structure -Krioukov et al (2008)

- Measurements of Internet are Gromov negatively curved Baryshnikov (2002)
- Curvature of co-links interpreted as thematic layers in WWW Eckmann and Moses (2002)

Question: Has anyone made this observation precise?

Hyperbolic Application: Clustering and Community Structure

Hyperbolic properties at large size scales:

- (Degree-weighted) expansion at large size-scales
- Degree heterogeneity

Local pockets of structure on hyperbolic scaffolding.

• (Traditionally-conceptualized) communities get worse and worse as they get larger and larger



Implications: for Community Detection

Linear (Low-rank) methods

If Gaussian, then low-rank space is good.

• Kernel (non-linear) methods

If low-dimensional manifold, then kernels are good

Hierarchical methods

Top-down and botton-up -- common in the social sciences

Graph partitioning methods

Define "edge counting" metric -- conductance, expansion, modularity, etc. -- in interaction graph, then optimize!

(Good and large) network communities, at least when formalized i.t.o. this bicriterion, don't really

/exist in these graphs!!

"It is a matter of common experience that communities exist in networks ... Although not precisely defined, communities are usually thought of as sets of nodes with better connections amongst its members than with the rest of the world."

Comparison with "Ground truth" (1 of 2)

Networks with "ground truth" communities:

- LiveJournal12:
 - users create and explicitly join on-line groups
- CA-DBLP:
 - publication venues can be viewed as communities
- AmazonAllProd:
 - each item belongs to one or more hierarchically organized categories, as defined by Amazon
- AtM-IMDB:
 - countries of production and languages may be viewed as communities (thus every movie belongs to exactly one community and actors belongs to all communities to which movies in which they appeared belong)

Comparison with "Ground truth" (2 of 2) 10⁰ 10⁰ 10⁻¹ ϕ (conductance) φ (conductance) 10⁻¹ 10⁻² 10⁻² 10⁻³ 10⁻⁴ 10⁻³ 10^{0} 10^{2} 10³ 10⁰ 10² 10^{3} 10^{1} 10⁴ 10⁵ 10^{1} 10^{4} 10⁵ n (number of nodes in the cluster) n (number of nodes in the cluster) LiveJournal **CA-DBLP** 10⁰ 10⁰ ϕ (conductance) ϕ (conductance) 10⁻¹ 10⁻¹ 10⁻² 10⁻² 10⁻³ 10⁻³ 10⁰ 10⁵ 10^{2} 10³ 10⁶ 10⁰ 10² 10³ 10⁵ 10^{4} 10^{1} 10⁴ 10^{1} n (number of nodes in the cluster) n (number of nodes in the cluster) AtM-IMDB AmazonAllProd

Implications: for Data Analysis and ML

Principled and scalable algorithmic exploratory analysis tools:

• spectral vs. flow vs. combinations; local vs. global vs. improvement; etc.

Doing inference directly on data graphs, and machine learning in complex data environments:

• don't do inference on feature vectors with hyperplanes in a vector space

• need methods to do it in high-variability, *only approximately* lowdimensional, tree-like or expander-like environments.

Implicit regularization via approximate computation:

• spectral vs. flow vs. combinations; local vs. global vs. improvement; etc.

Conclusions (1 of 2)

- Geometric tools for experimentally "probing" large social and information graphs: geometry ~ inference
- Tools for coupling local properties (often lowdimensional) and global properties (expander-like)
- Real informatics graphs -- very different than small commonly-studied graphs and existing generative models

Conclusions (2 of 2)

• Validation is difficult - if you have a clean validation and/or a pretty picture, you're looking at unrealistic network data!

• **Important:** even if you do not care about communities, conductance, hyperbolicity, etc., these empirical facts place very severe constraints on the types of models and types of analysis tools that are appropriate.