Approximate computation and implicit regularization for very large-scale data analysis

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Algorithmic vs. Statistical Perspectives

Lambert (2000); Mahoney "Algorithmic and Statistical Perspectives on Large-Scale Data Analysis" (2010)

Computer Scientists

• *Data*: are a record of everything that happened.
• *Goal*: process the data to find interesting patterns and associations.
• *Methodology*: Develop approximation algorithms under different models of data access since the goal is typically computationally hard.

Statisticians (and Natural Scientists, etc)

• *Data*: are a particular random instantiation of an underlying process describing unobserved patterns in the world.
• *Goal*: is to extract information about the world from noisy data.
• *Methodology*: Make inferences (perhaps about unseen events) by positing a model that describes the random variability of the data around the deterministic model.

Perspectives are NOT incompatible

- Statistical/probabilistic ideas are central to recent work on developing improved randomized algorithms for matrix problems.

- Intractable optimization problems on graphs/networks yield to approximation when assumptions are made about network participants.

- In boosting (a statistical technique that fits an additive model by minimizing an objective function with a method such as gradient descent), the computation parameter (i.e., the number of iterations) also serves as a regularization parameter.

But they are VERY different **paradigms**

Statistics, natural sciences, scientific computing, etc:

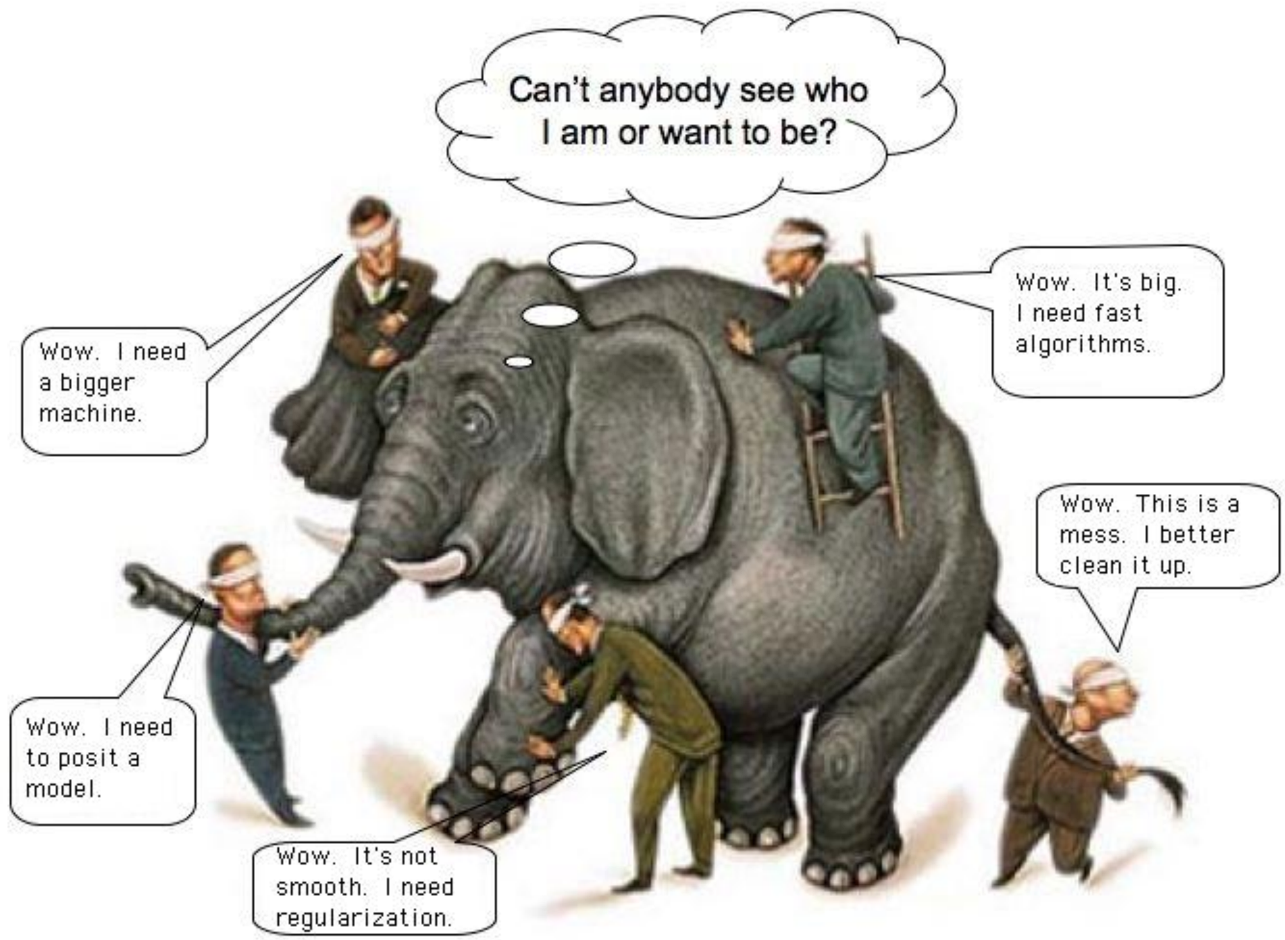
- Problems often involve computation, but the study of computation *per se* is secondary
- Only makes sense to develop algorithms for well-posed* problems
- First, write down a model, and think about computation later

Computer science:

- Easier to study computation *per se* in discrete settings, e.g., Turing machines, logic, complexity classes
- Theory of algorithms divorces computation from data
- First, run a fast algorithm, and ask what it means later

*Solution exists, is unique, and varies continuously with input data

How do we view BIG data?



Anecdote 1:
Randomized Matrix Algorithms

Mahoney "Algorithmic and Statistical Perspectives on Large-Scale Data Analysis" (2010)
Mahoney "Randomized Algorithms for Matrices and Data" (2011)

Theoretical origins

- theoretical computer science, convex analysis, etc.
- Johnson-Lindenstrauss
- Additive-error algs
- Good worst-case analysis
- No statistical analysis

Practical applications

- NLA, ML, statistics, data analysis, genetics, etc
- Fast JL transform
- Relative-error algs
- Numerically-stable algs
- Good statistical properties

How to "bridge the gap"?

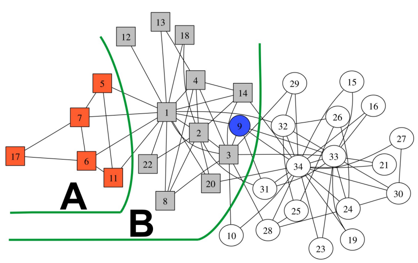
- decouple randomization from linear algebra
- importance of statistical leverage scores!

Anecdote 2: Communities in large informatics graphs

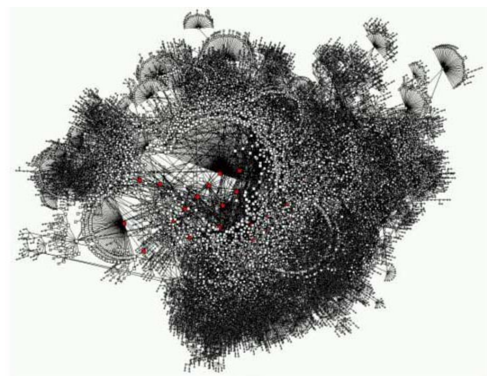
Mahoney "Algorithmic and Statistical Perspectives on Large-Scale Data Analysis" (2010)
Leskovec, Lang, Dasgupta, & Mahoney "Community Structure in Large Networks ..." (2009)

Data are expander-like at large size scales !!!

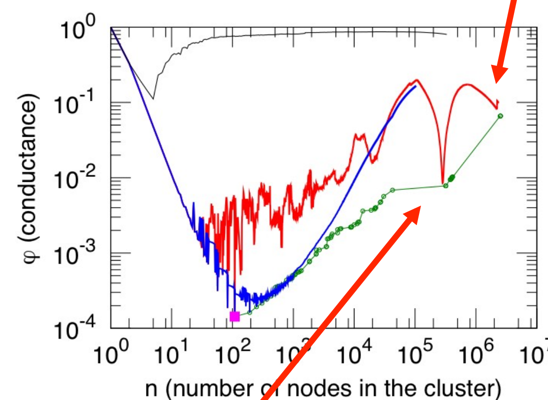
People imagine social networks to look like:



Real social networks actually look like:



Size-resolved conductance (degree-weighted expansion) plot looks like:



There do not exist good large clusters in these graphs !!!

How do we know this plot is "correct"?

- (since computing conductance is intractable)
- Algorithmic Result (ensemble of sets returned by different approximation algorithms are very different)
- Statistical Result (Spectral provides more meaningful communities than flow)
- Lower Bound Result; Structural Result; Modeling Result; Etc.

Lessons from the anecdotes

Mahoney "Algorithmic and Statistical Perspectives on Large-Scale Data Analysis" (2010)

We are being forced to engineer a union between two very different worldviews on what are fruitful ways to view the data

- in spite of our best efforts *not* to

Often fruitful to consider the statistical properties implicit in worst-case algorithms

- rather that *first* doing statistical modeling and *then* doing applying a computational procedure as a black box
- for both anecdotes, this was *essential* for leading to "useful theory"

How to extend these ideas to "bridge the gap" b/w the theory and practice of MMDS (Modern Massive Data Set) analysis.

- **QUESTION:** Can we identify a/the *concept at the heart of the algorithmic-statistical disconnect* and then drill-down on it?

Outline and overview

Preamble: algorithmic & statistical perspectives

General thoughts: data, algorithms, and explicit & implicit regularization

Approximate first nontrivial eigenvector of Laplacian

- Three random-walk-based procedures (heat kernel, PageRank, truncated lazy random walk) are *implicitly* solving a regularized optimization *exactly*!

Spectral versus flow-based algs for graph partitioning

- Theory says each regularizes in different ways; empirical results agree!

Weakly-local and strongly-local graph partitioning methods

- Operationally like L1-regularization and already used in practice!

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Thoughts on models of data (1 of 2)

Data are whatever data are

• records of banking/financial transactions, hyperspectral medical/astronomical images, electromagnetic signals in remote sensing applications, DNA microarray/SNP measurements, term-document data, search engine query/click logs, user interactions on social networks, corpora of images, sounds, videos, etc.

To do something useful, you must *model the data*

Two criteria when choosing a data model

• (data acquisition/generation side): want a structure that is "close enough" to the data that you don't do too much "damage" to the data

• (downstream/analysis side): want a structure that is at a "sweet spot" between descriptive flexibility and algorithmic tractability

Thoughts on models of data (2 of 2)

Examples of data models:

• *Flat tables and the relational model:* one or more two-dimensional arrays of data elements, where different arrays can be related by predicate logic and set theory.

• *Graphs, including trees and expanders:* G=(V,E), with a set of nodes V that represent "entities" and edges E that represent "interactions" between pairs of entities.

• *Matrices, including SPSD matrices:* m "objects," each of which is described by n "features," i.e., an n-dimensional Euclidean vector, gives an m x n matrix A.

Much modern data are relatively-unstructured; matrices and graphs are often useful, especially when traditional databases have problems.

Relationship b/w algorithms and data (1 of 3)

Before the digital computer:

• Natural sciences rich source of problems, statistical methods developed to solve those problems

• *Very* important notion: well-posed (well-conditioned) problem: solution exists, is unique, and is continuous w.r.t. problem parameters

• *Simply doesn't make sense to solve ill-posed problems*

Advent of the digital computer:

• Split in (yet-to-be-formed field of) "Computer Science"

• Based on application (scientific/numerical computing vs. business/ consumer applications) as well as tools (continuous math vs. discrete math)

• *Two very different perspectives on relationship b/w algorithms and data*

Relationship b/w algorithms and data (2 of 3)

Two-step approach for "numerical" problems

- Is problem well-posed/well-conditioned?
- If no, replace it with a well-posed problem. (Regularization!)
- If yes, design a stable algorithm.

View Algorithm A as a function f

- Given x, it tries to compute y but actually computes y*
- Forward error: $\Delta y = y^* - y$
- Backward error: smallest Δx s.t. $f(x+\Delta x) = y^*$
- Forward error ≤ Backward error * condition number
- *Backward-stable algorithm provides accurate solution to well-posed problem!*

Relationship b/w algorithms and data (3 of 3)

One-step approach for study of computation, *per se*

- Concept of computability captured by 3 seemingly-different discrete processes (recursion theory, λ-calculus, Turing machine)
- Computable functions have internal structure (P vs. NP, NP-hardness, etc.)
- Problems of practical interest are "intractable" (e.g., NP-hard vs. poly(n), or $O(n^3)$ vs. $O(n \log n)$)

Modern Theory of Approximation Algorithms

- provides forward-error bounds for worst-cast input
- worst case in two senses: (1) for all possible input & (2) i.t.o. relatively-simple complexity measures, but independent of "structural parameters"
- get bounds by "relaxations" of IP to LP/SDP/etc., i.e., a "nicer" place

Statistical regularization (1 of 3)

Regularization in statistics, ML, and data analysis

- arose in integral equation theory to "solve" ill-posed problems
- computes a better or more "robust" solution, so better inference
- involves making (explicitly or implicitly) assumptions about data
- provides a trade-off between "solution quality" versus "solution niceness"
- often, heuristic approximation procedures have regularization properties as a "side effect"
- lies at *the heart of the disconnect between the "algorithmic perspective" and the "statistical perspective"*

Statistical regularization (2 of 3)

Usually *implemented* in 2 steps:

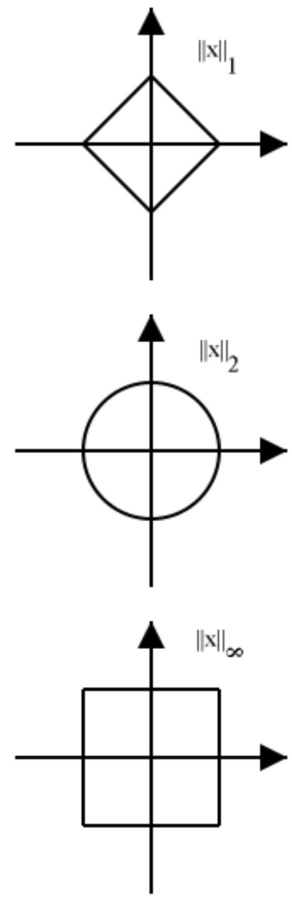
- add a norm constraint (or "geometric capacity control function") $g(x)$ to objective function $f(x)$

- solve the modified optimization problem

$$x' = \mathrm{argmin}_x \; f(x) + \lambda \, g(x)$$

Often, this is a "harder" problem, e.g., L1-regularized L2-regression

$$x' = \mathrm{argmin}_x \; ||Ax-b||_2 + \lambda \, ||x||_1$$



Statistical regularization (3 of 3)

Regularization is often observed as a side-effect or by-product of other design decisions

- “binning,” “pruning,” etc.
- “truncating” small entries to zero, “early stopping” of iterations
- approximation algorithms and heuristic approximations engineers do to implement algorithms in large-scale systems

BIG question: Can we formalize the notion that/when approximate computation can *implicitly* lead to “better” or “more regular” solutions than exact computation?

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Notation for weighted undirected graph

- vertex set $V = \{1, \ldots, n\}$
- edge set $E \subset V \times V$
- edge weight function $w : E \rightarrow R_+$
- degree function $d : V \rightarrow R_+$, $d(u) = \sum_v w(u, v)$
- diagonal degree matrix $D \in R^{V \times V}$, $D(v, v) = d(v)$
- combinatorial Laplacian $L_0 = D - W$
- normalized Laplacian $L = D^{-1/2} L_0 D^{-1/2}$

Approximating the top eigenvector

Basic idea: Given an SPSD (e.g., Laplacian) matrix A,

- Power method starts with v_0, and iteratively computes

$$v_{t+1} = Av_t / ||Av_t||_2 \quad .$$

- Then, $v_t = \Sigma_i \gamma_i^t v_i \rightarrow v_1$.

- If we truncate after (say) 3 or 10 iterations, still have some mixing from other eigen-directions

What objective does the exact eigenvector optimize?

- Rayleigh quotient $R(A,x) = x^T A x / x^T x$, for a *vector* x.
- But can also express this as an SDP, for a SPSD *matrix* X.
- (We will put regularization on this SDP!)

Views of approximate spectral methods

Three common procedures (L=Laplacian, and M=r.w. matrix):

- Heat Kernel:

$$H_t = \exp(-tL) = \sum_{k=0}^{\infty} \frac{(-t)^k}{k!} L^k$$

- PageRank:

$$\pi(\gamma, s) = \gamma s + (1-\gamma) M \pi(\gamma, s)$$

$$R_\gamma = \gamma \left(I - (1-\gamma) M\right)^{-1}$$

- q-step Lazy Random Walk:

$$W_\alpha^q = (\alpha I + (1-\alpha) M)^q$$

Question: Do these "*approximation* procedures" *exactly* optimizing some regularized objective?

Two versions of spectral partitioning

VP:

$$\begin{aligned} \text{min.} \quad & x^T L_G x \\ \text{s.t.} \quad & x^T L_{K_n} x = 1 \\ & < x, 1 >_D = 0 \end{aligned}$$

↓

R-VP:

$$\begin{aligned} \text{min.} \quad & x^T L_G x + \lambda f(x) \\ \text{s.t.} \quad & constraints \end{aligned}$$

Two versions of spectral partitioning

VP: ⟷ **SDP:**

$$\begin{aligned} \text{min.} \quad & x^T L_G x \\ \text{s.t.} \quad & x^T L_{K_n} x = 1 \\ & < x, 1 >_D = 0 \end{aligned}$$

$$\begin{aligned} \text{min.} \quad & L_G \circ X \\ \text{s.t.} \quad & L_{K_n} \circ X = 1 \\ & X \succeq 0 \end{aligned}$$

↓ ↓

R-VP:

$$\begin{aligned} \text{min.} \quad & x^T L_G x + \lambda f(x) \\ \text{s.t.} \quad & constraints \end{aligned}$$

R-SDP:

$$\begin{aligned} \text{min.} \quad & L_G \circ X + \lambda F(X) \\ \text{s.t.} \quad & constraints \end{aligned}$$

A simple theorem

Mahoney and Orecchia (2010)

$$\text{(F,}\eta\text{)-SDP} \quad \min \quad L \bullet X + \frac{1}{\eta} \cdot F(X)$$
$$\text{s.t.} \quad I \bullet X = 1$$
$$X \succeq 0$$

Modification of the usual SDP form of spectral to have regularization (but, on the matrix X, not the vector x).

Theorem: Let G be a connected, weighted, undirected graph, with normalized Laplacian L. Then, the following conditions are sufficient for $X^\star$ to be an optimal solution to (F,η)-SDP.

- $X^\star = (\nabla F)^{-1}(\eta \cdot (\lambda^* I - L))$, for some $\lambda^* \in R$,
- $I \bullet X^\star = 1$,
- $X^\star \succeq 0$.

Three simple corollaries

$F_H(X) = Tr(X \log X) - Tr(X)$ (i.e., generalized entropy)

gives scaled Heat Kernel matrix, with $t = \eta$

$F_D(X) = -\text{logdet}(X)$ (i.e., Log-determinant)

gives scaled PageRank matrix, with $t \sim \eta$

$F_p(X) = (1/p)||X||_p^p$ (i.e., matrix p-norm, for $p>1$)

gives Truncated Lazy Random Walk, with $\lambda \sim \eta$

(F(•) specifies the algorithm; "number of steps" specifies the η)

Answer: These "approximation procedures" compute regularized versions of the Fiedler vector *exactly*!

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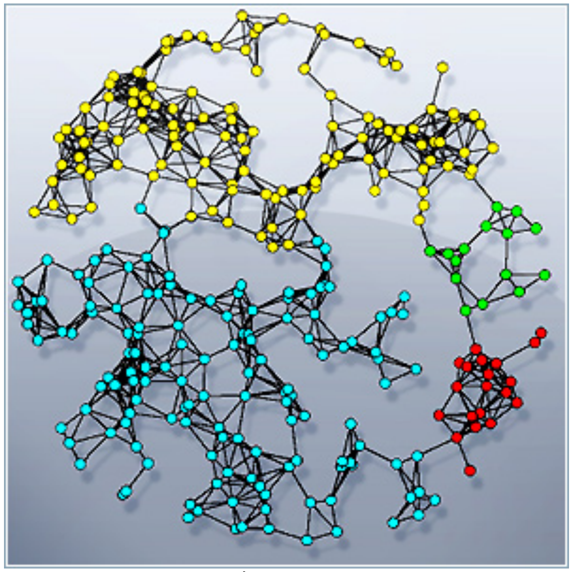
Graph partitioning

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)) (conductance or N-Cuts)

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

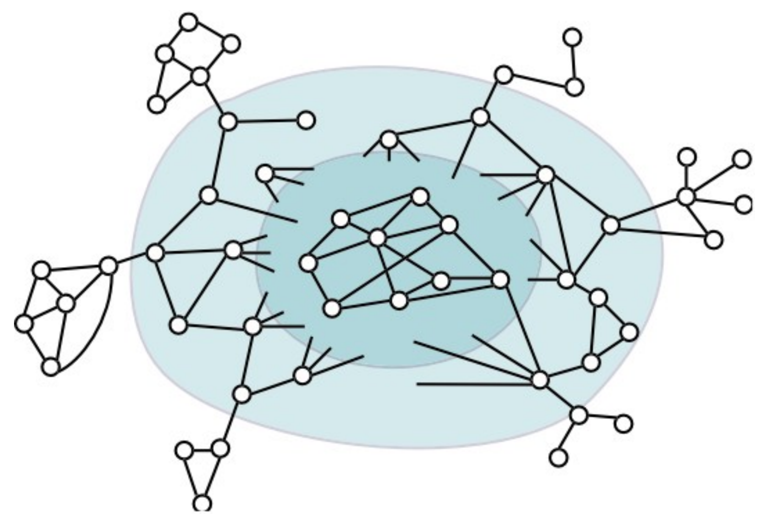
Networks and networked data

Lots of "networked" data!!

- technological networks
  - AS, power-grid, road networks
- biological networks
  - food-web, protein networks
- social networks
  - collaboration networks, friendships
- information networks
  - co-citation, blog cross-postings, advertiser-bidded phrase graphs...
- language networks
  - semantic networks...
- ...

Interaction graph model of networks:

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



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]

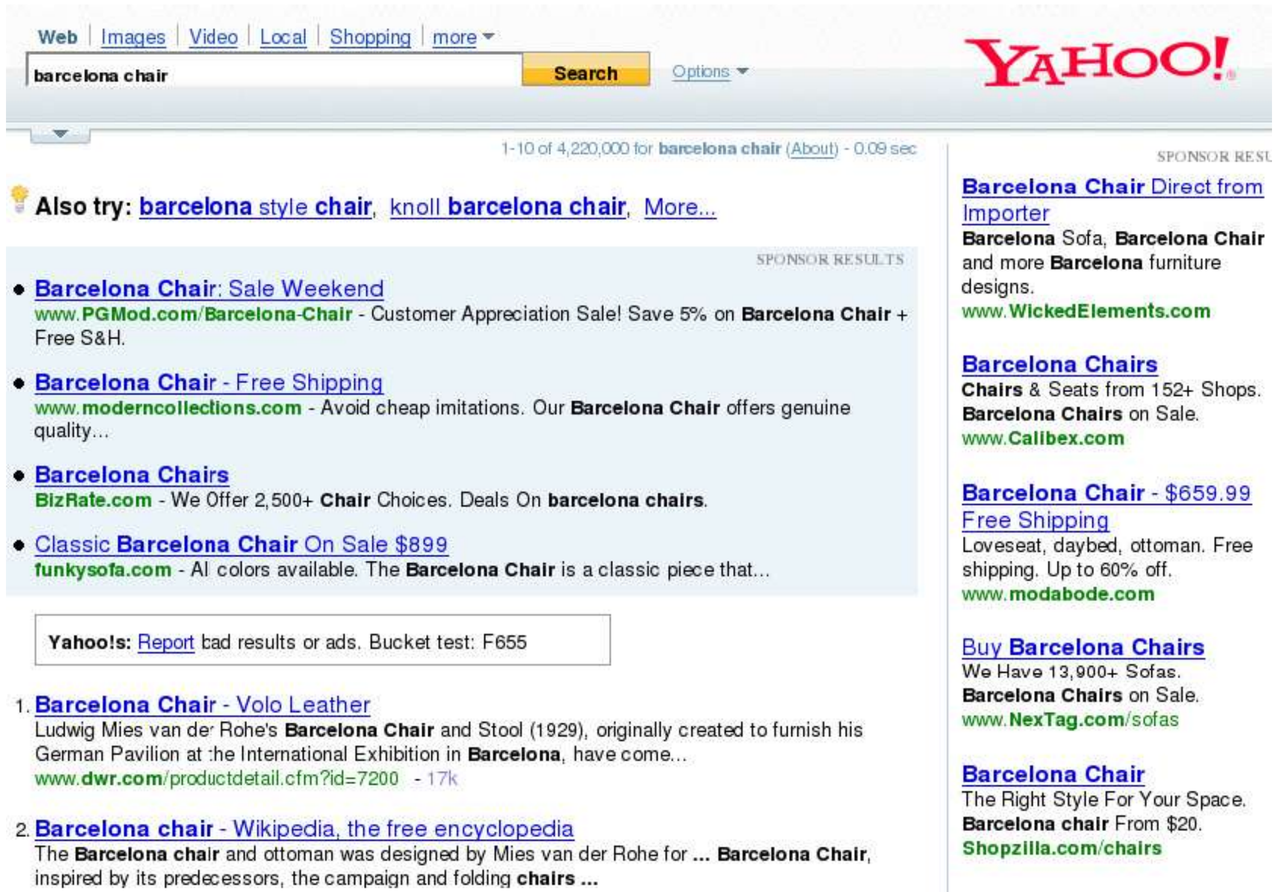
Table 1: Some of the network datasets we studied.

Motivation: Sponsored ("paid") Search

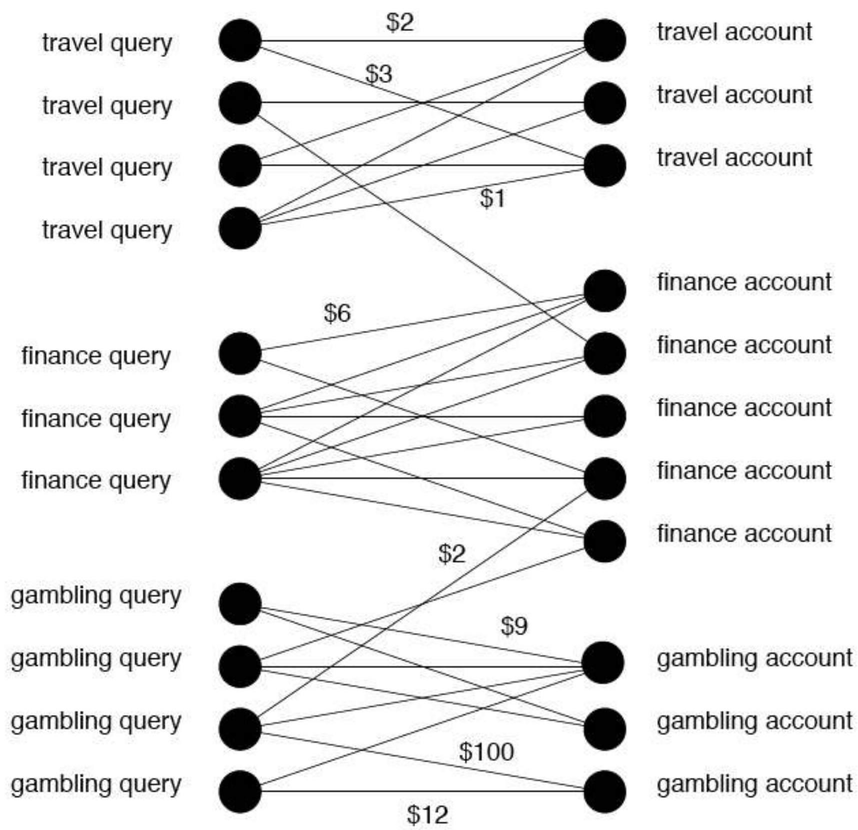
Text based ads driven by user specified query

The process:

- Advertisers bids on query phrases.
- Users enter query phrase.
- Auction occurs.
- Ads selected, ranked, displayed.
- When user clicks, advertiser pays!



Bidding and Spending Graphs



A "social network" with "term-document" aspects.

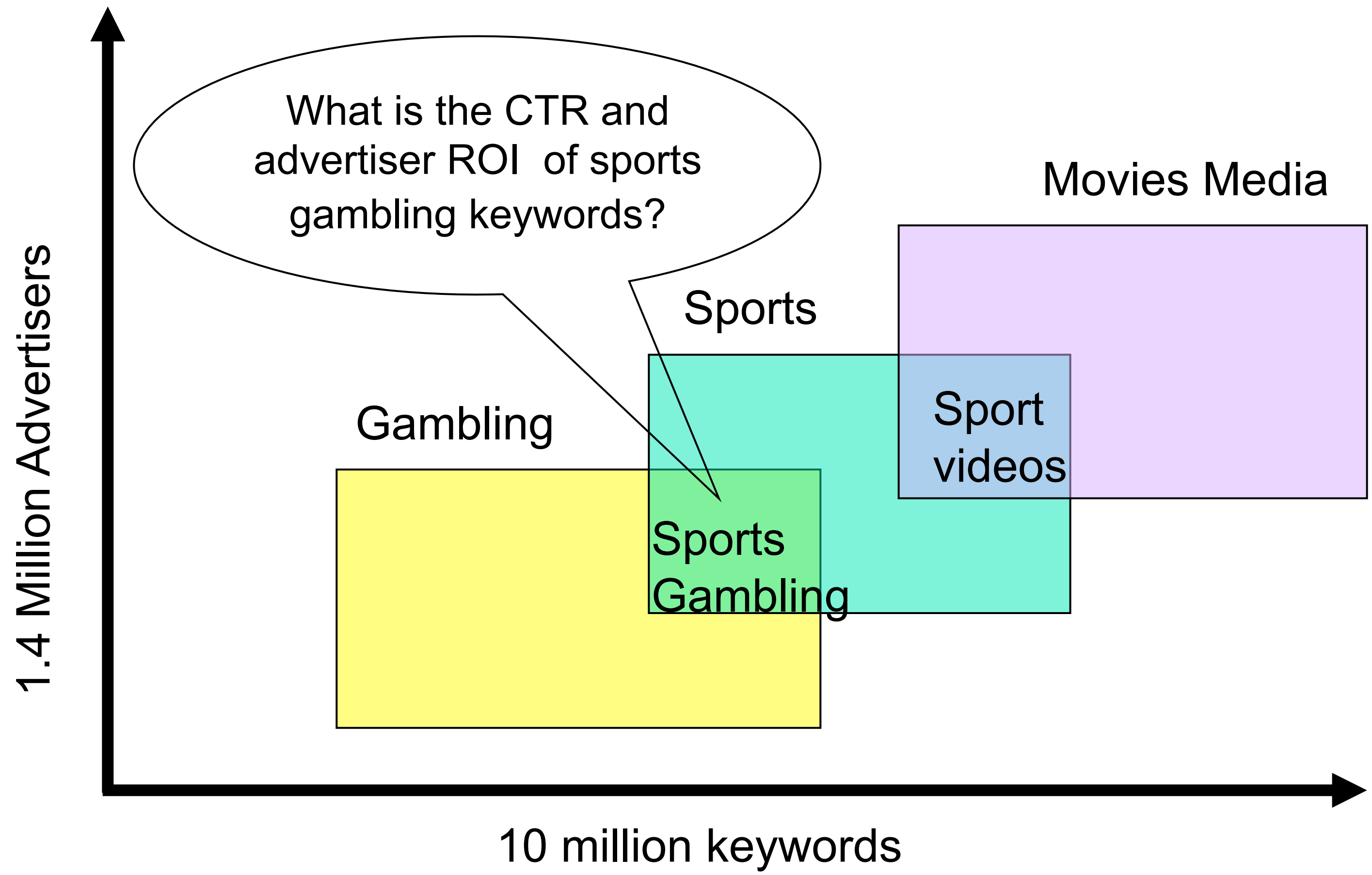
Uses of Bidding and Spending graphs:

- "deep" micro-market identification.
- improved query expansion.

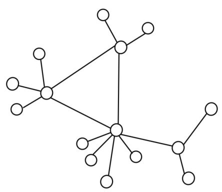
More generally, user segmentation for behavioral targeting.

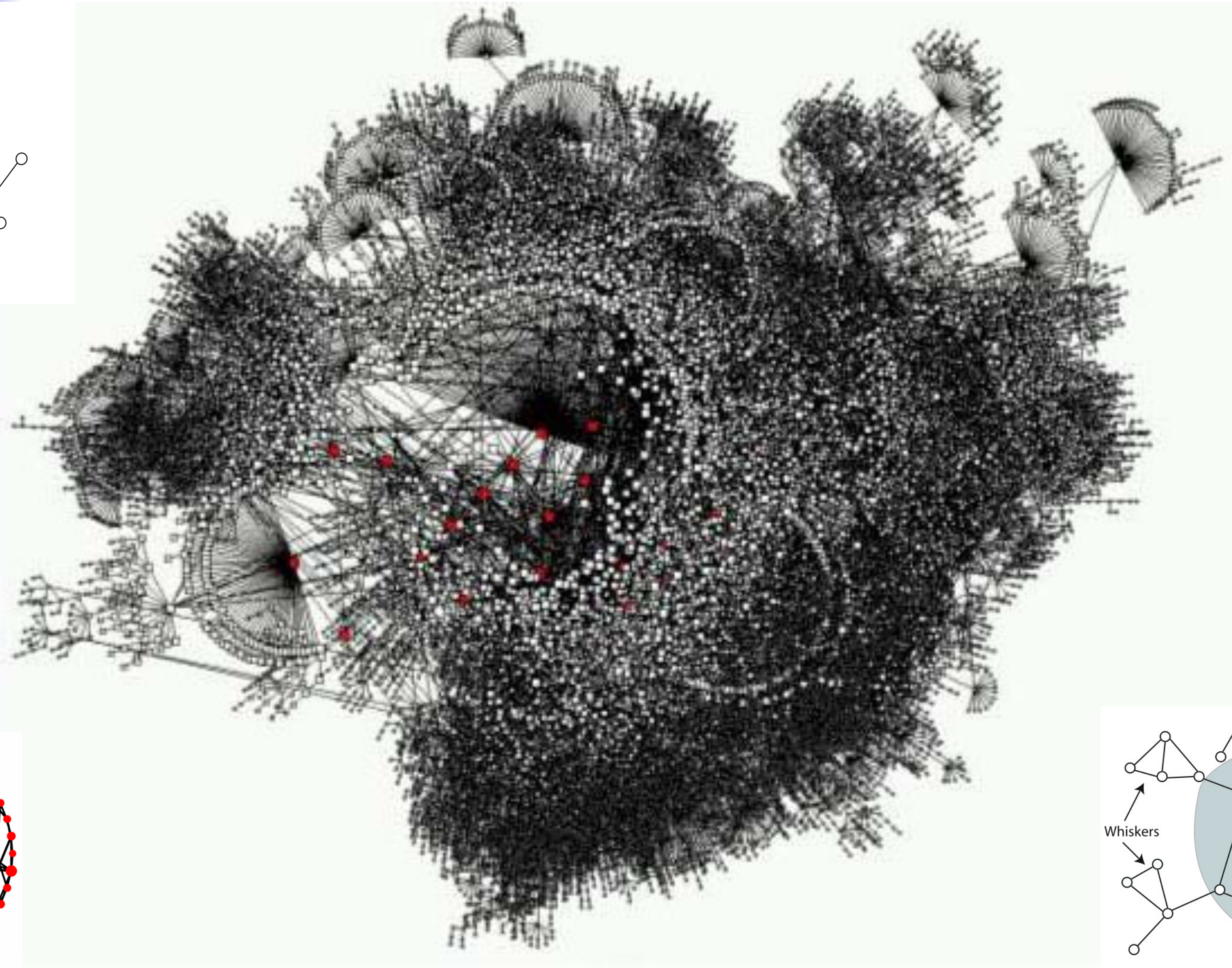
Micro-markets in sponsored search

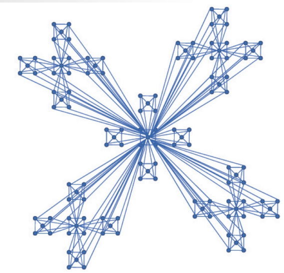
Goal: Find *isolated* markets/clusters with *sufficient money/clicks* with *sufficient coherence.*
Ques: Is this even possible?

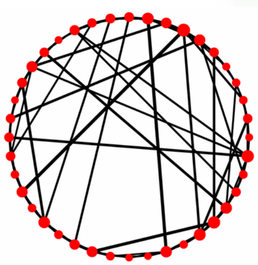


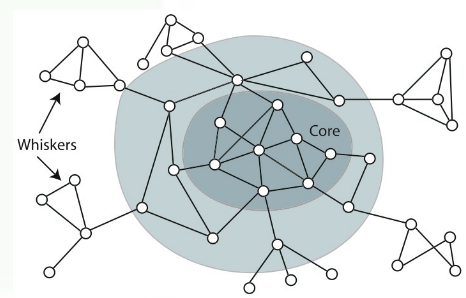
What do these networks "look" like?











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 multi-commodity version of max-flow-min-cut ideas

*Comes with *strong* underlying theory to guide heuristics.

Comparison of “spectral” versus “flow”

Spectral:

- Compute an eigenvector
- “Quadratic” worst-case bounds
- Worst-case achieved -- on “long stringy” graphs
- Worse-case is “local” property
- Embeds you on a line (or K_n)

Flow:

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

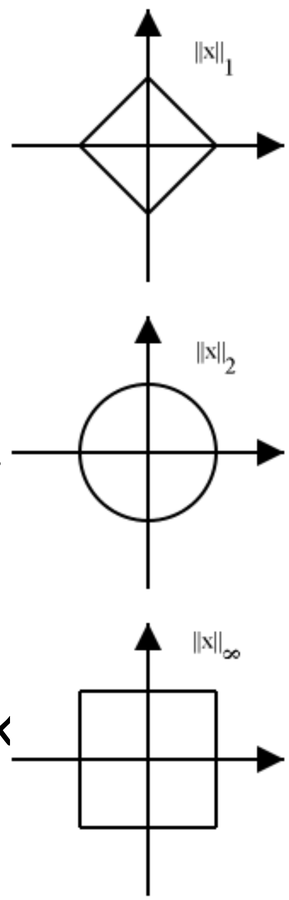
Two methods -- complementary strengths and weaknesses

- What we compute is determined at least as much by as the approximation algorithm as by objective function.

Explicit versus implicit geometry

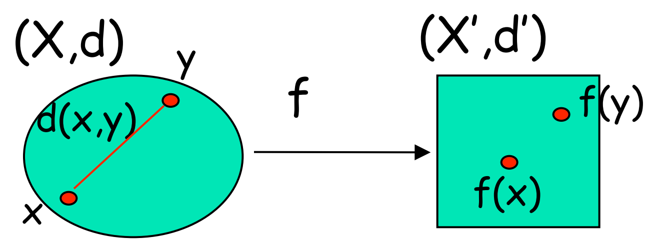
Explicitly-imposed geometry

- Traditional regularization uses *explicit* norm constraint to make sure solution vector is "small" and not-too-complex

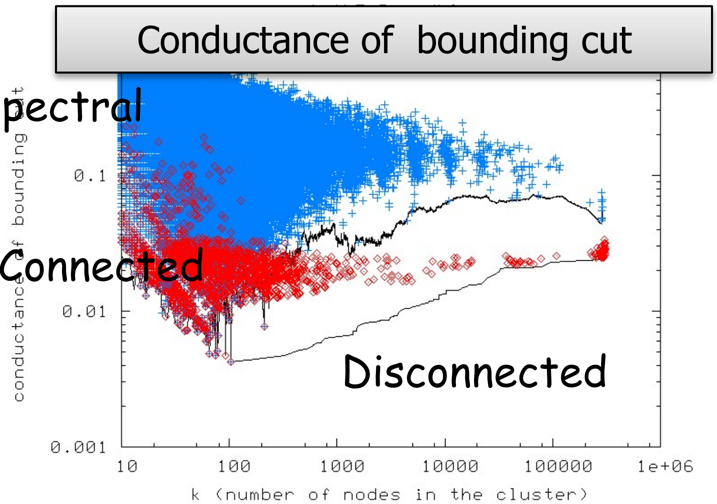


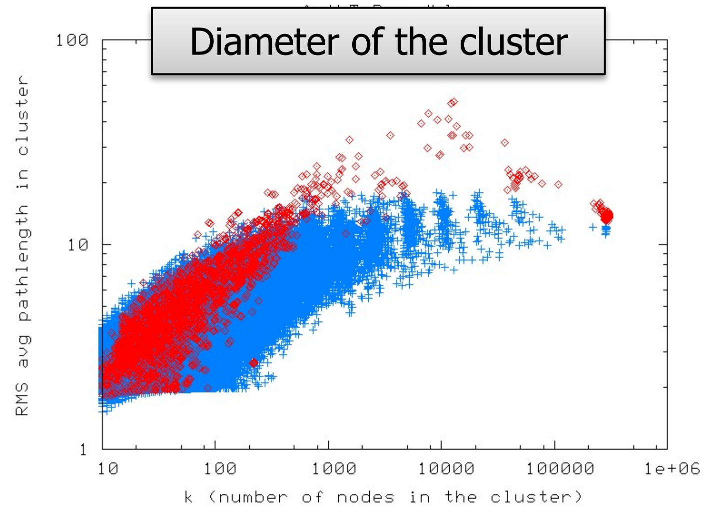
Implicitly-imposed geometry

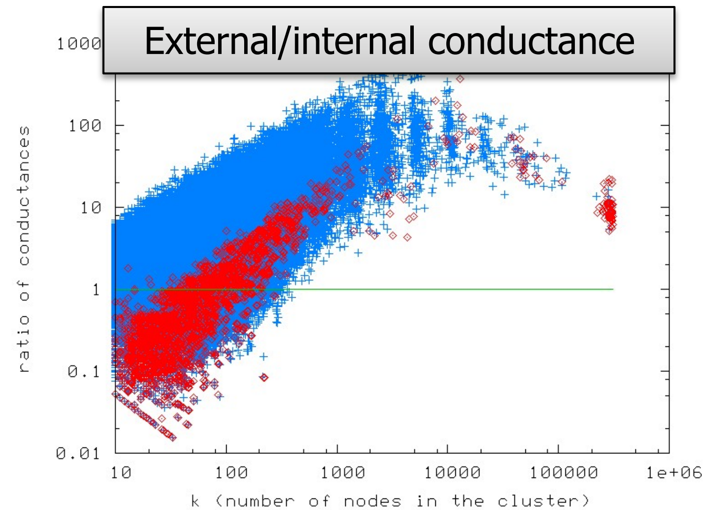
- Approximation algorithms *implicitly* embed the data in a "nice" metric/geometric place and then round the solution.



Regularized and non-regularized communities (1 of 2)





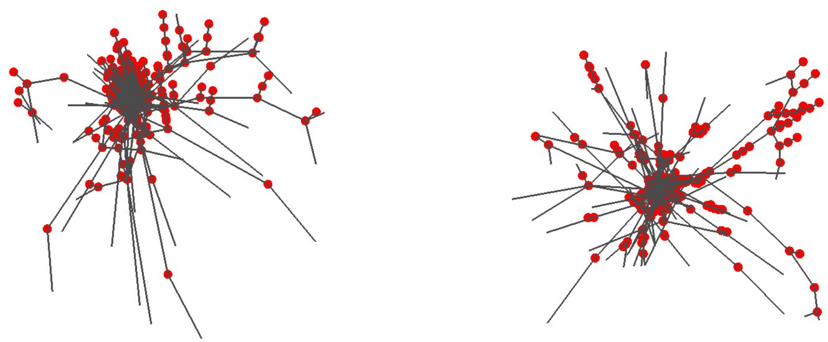


Lower is good

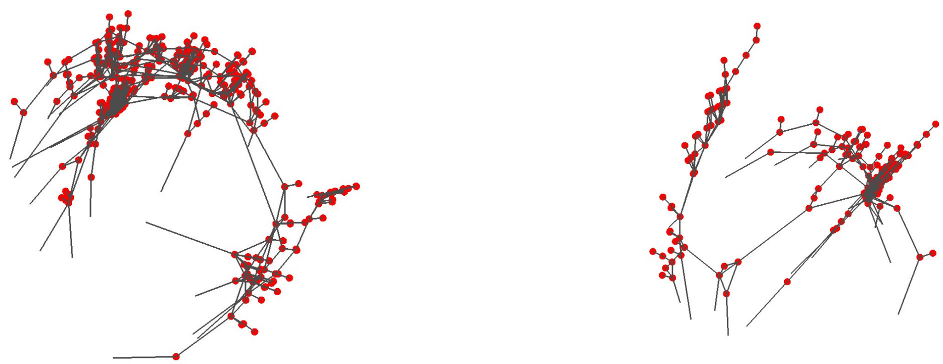
- Metis+MQI - a Flow-based method (red) gives sets with better conductance.
- Local Spectral (blue) gives tighter and more well-rounded sets.

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:



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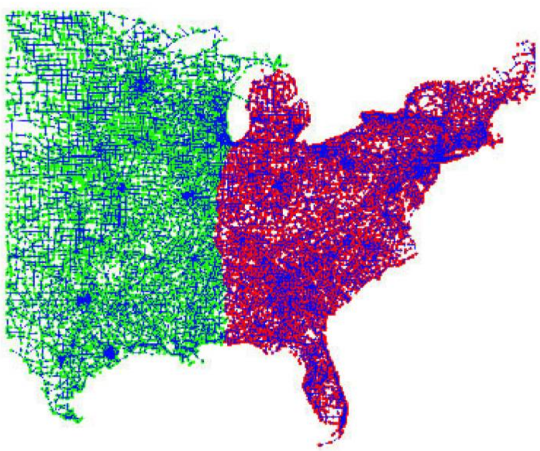
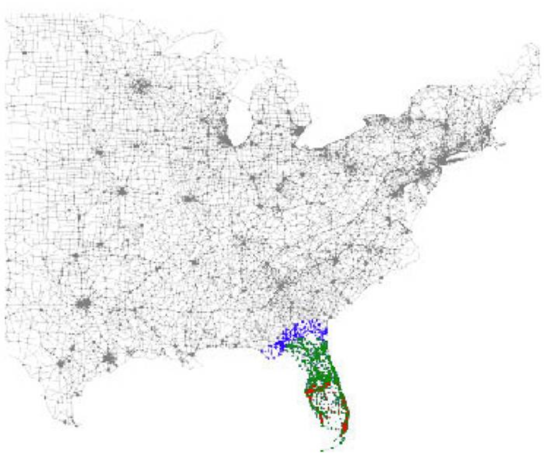
Computing locally-biased partitions

Often want clusters "near" a pre-specified set of nodes:

- Large social graphs have good small clusters, don't have good large clusters
- Might have domain knowledge, so find "semi-supervised" clusters
- As algorithmic primitives, e.g., to solve linear equations fast.





Recall global spectral graph partitioning

The basic optimization problem:

$$\begin{aligned} \text{minimize} \quad & x^T L_G x \\ \text{s.t.} \quad & \langle x, x \rangle_D = 1 \\ & \langle x, 1 \rangle_D = 0 \end{aligned}$$

• Relaxation of:

$$\phi(G) = \min_{S \subset V} \frac{E(S, \bar{S})}{Vol(S)Vol(\bar{S})}$$

• Solvable via the eigenvalue problem:

$$\mathcal{L}_G y = \lambda_2(G) y$$

• Sweep cut of second eigenvector yields:

$$\lambda_2(G)/2 \leq \phi(G) \leq \sqrt{8\lambda_2(G)}$$

Idea to compute locally-biased partitions:

- Modify this objective with a locality constraint
- Show that some/all of these nice properties still hold locally

Local spectral partitioning *ansatz*

Mahoney, Orecchia, and Vishnoi (2010)

Primal program:

$$\begin{aligned} \text{minimize} \quad & x^T L_G x \\ \text{s.t.} \quad & < x, x >_D = 1 \\ & < x, s >_D^2 \geq \kappa \end{aligned}$$

Interpretation:

- Find a cut well-correlated with the seed vector s.
- If s is a single node, this relaxes:

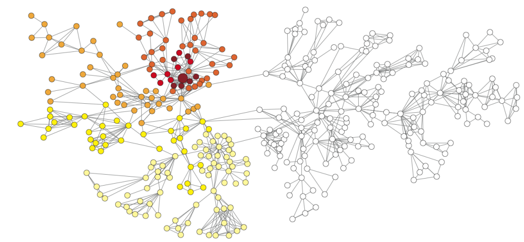
$$\min_{S \subset V, s \in S, |S| \leq 1/k} \frac{E(S, \bar{S})}{Vol(S) Vol(\bar{S})}$$

Dual program:

$$\begin{aligned} \max \quad & \alpha - \beta(1 - \kappa) \\ \text{s.t.} \quad & L_G \succeq \alpha L_{K_n} - \beta \left(\frac{L_{K_T}}{\text{vol}(\bar{T})} + \frac{L_{K_{\bar{T}}}}{\text{vol}(T)} \right) \\ & \beta \geq 0 \end{aligned}$$

Interpretation:

- Embedding a combination of scaled complete graph K_n and complete graphs T and $\underline{T}$ (K_T and $K_{\underline{T}}$) - where the latter encourage cuts near (T,$\underline{T}$).



Main theoretical results

Mahoney, Orecchia, and Vishnoi (2010)

Theorem: If x^* is an optimal solution to LocalSpectral,

(*) it is a Generalized Personalized PageRank vector, and can be computed as solution to a set of linear equations;

Fast running time guarantee.

(*) one can find a cut of conductance $\leq 8\lambda(G,s,\kappa)$ in time $O(n \lg n)$ with sweep cut of x^*;

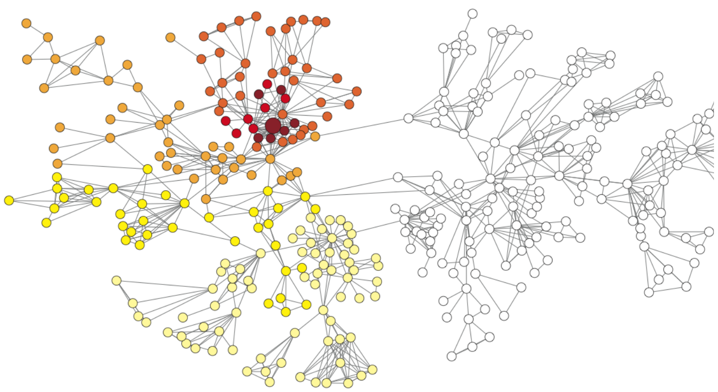
Upper bound, as usual from sweep cut & Cheeger.

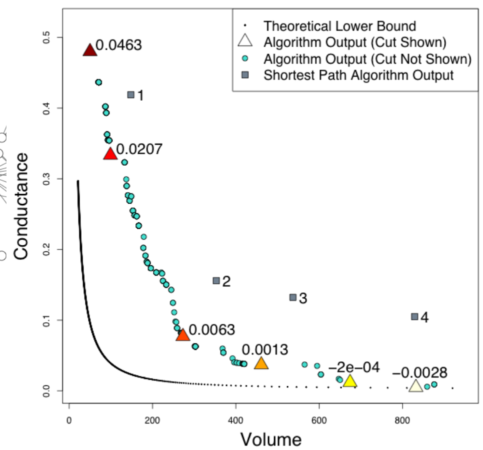
(*) For all sets of nodes T s.t. $\kappa' := \langle s, s_T \rangle_D^2$, we have: $\phi(T) \geq \lambda(G,s,\kappa)$ if $\kappa \leq \kappa'$, and $\phi(T) \geq (\kappa'/\kappa)\lambda(G,s,\kappa)$ if $\kappa' \leq \kappa$.

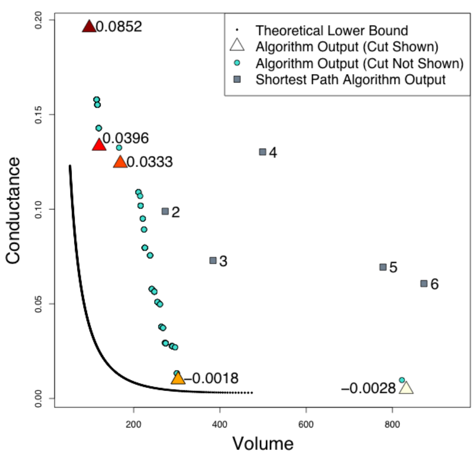
Lower bound: Spectral version of flow-improvement algs.

Illustration on small graphs

Mahoney, Orecchia, and Vishnoi (2010)







- Similar results if we do local random walks, truncated PageRank, and heat kernel diffusions.
- Often, it finds "worse" quality but "nicer" partitions than flow-improve methods. (Tradeoff we'll see later.)

A somewhat different approach

Strongly-local spectral methods

- ST04: truncated "local" random walks to compute locally-biased cut
- ACL06: approximate locally-biased PageRank vector computations
- Chung08: approximate heat-kernel computation to get a vector

These are the diffusion-based procedures

- that we saw before
- *except truncate/round/clip/push small things to zero*
- starting with localized initial condition

Also get provably-good local version of global spectral

What's the connection?

"Optimization" approach:

- Well-defined objective f
- Weakly local (touch all nodes), so good for medium-scale problems
- Easy to use

"Operational" approach*:

- *Very* fast algorithm
- Strongly local (clip/truncate small entries to zero), good for large-scale
- Very difficult to use

* *Informally, optimize f+λg (... almost formally!):* steps are structurally-similar to the steps of how, e.g., L1-regularized L2 regression algorithms, implement regularization

More importantly,

- This "operational" approach is *already* being adopted in PODS/VLDB/SIGMOD/KDD/WWW environments!
- Let's make the regularization explicit—and know what we compute!

Looking forward ...

A common *modus operandi* in many (really*) large-scale applications is:

- Run a procedure that bears some resemblance to the procedure you would run if you were to solve a given problem exactly
- Use the output in a way similar to how you would use the exact solution, or prove some result that is similar to what you could prove about the exact solution.

BIG Question: Can we make this more principled? E.g., can we "engineer" the approximations to solve (exactly but implicitly) some regularized version of the original problem---to do large scale analytics in a statistically more principled way?

*e.g., industrial production, publication venues like WWW, SIGMOD, VLDB, etc.

Conclusions

Regularization is:

- absent from CS, which historically has studied computation per se
- central to nearly area that applies algorithms to noisy data
- gets at the heart of the algorithmic-statistical “disconnect”

Approximate computation, *in and of itself*, can *implicitly* regularize:

- Theory & the empirical signatures in matrix *and* graph problems
- Solutions of approximation algorithms don’t need to be something we “settle for,” they can be “better” than the “exact” solution

In very large-scale analytics applications:

- Can we “engineer” database operations so “worst-case” approximation algorithms exactly solve regularized versions of original problem?
- I.e., can we get best of both worlds for very large-scale analytics?

MMDS Workshop on "Algorithms for Modern Massive Data Sets"

(http://mmds.stanford.edu)

at Stanford University, July 10-13, 2012

Objectives:

- Address algorithmic, statistical, and mathematical challenges in modern statistical data analysis.

- Explore novel techniques for modeling and analyzing massive, high-dimensional, and nonlinearly-structured data.

- Bring together computer scientists, statisticians, mathematicians, and data analysis practitioners to promote cross-fertilization of ideas.

Organizers: M. W. Mahoney, A. Shkolnik, G. Carlsson, and P. Drineas,

Registration is available now!