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Sandia National Laboratories

Solving Graph Laplacians for Complex Networks

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Outline

- Graph Laplacians
- Linear systems and preconditioners
- Normalization
- Empirical study with Trilinos
- Nearly-optimal combinatorial solvers
  - Kelner et al.'s simple iterative method
- Conclusions

Complex Networks: Numerical Computing

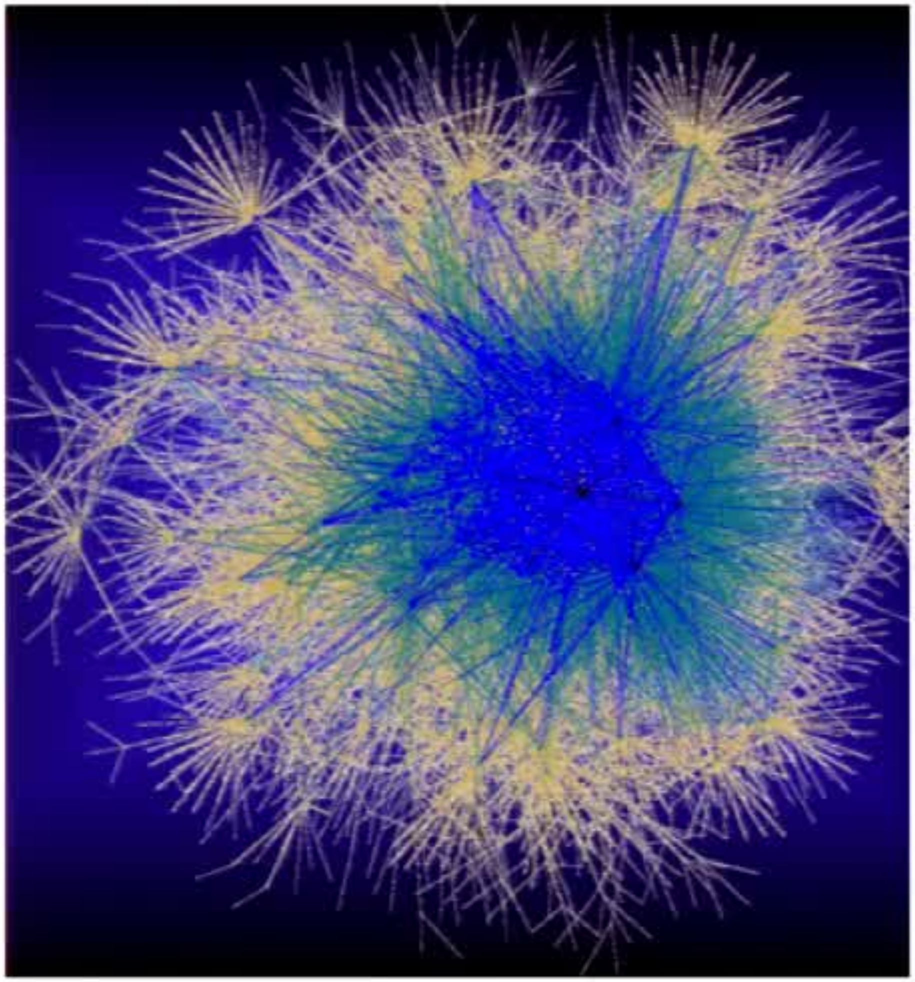
Complex networks often analyzed by

- Degree distribution
- Clustering coefficient
- Centrality metrics

Less attention on numerical linear algebra:

- Linear system: $Ax=b$
- Eigenproblem: $Ax = \lambda x$

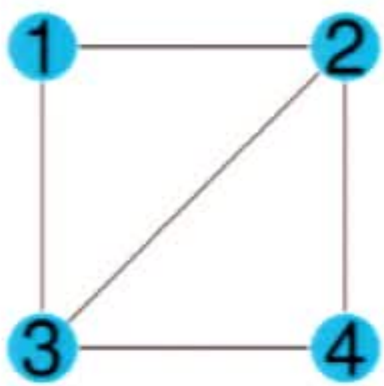
Well studied for PDEs, but not for complex networks.



BGP graph (credit: Richardson, Chung)
http://math.ucsd.edu/~fan/graphs/gallery

Matrices from Graphs

Symbol	Matrix
A	Adjacency matrix
D	Diagonal vertex degree matrix
L = D-A	Graph Laplacian
$L_N = D^{-1/2}(D-A)D^{-1/2}$	Normalized Laplacian



$$\begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 3 & -1 & -1 \\ -1 & -1 & 3 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix}$$

Solving Linear Systems

Different research communities, different approaches!

- Numerical linear algebra
  - Empirical focus
    - Analysis for model problems sufficient
  - Main application: discretizations of PDEs
  - Good and robust software for solving large systems
- CS Theory
  - Focus on theory and complexity
    - Worst-case analysis
  - Main target: graph Laplacians, SDD systems
  - Software not important (some Matlab codes)
- Network Science
  - Just a tool – don't care how it's done

Solvers and Preconditioners

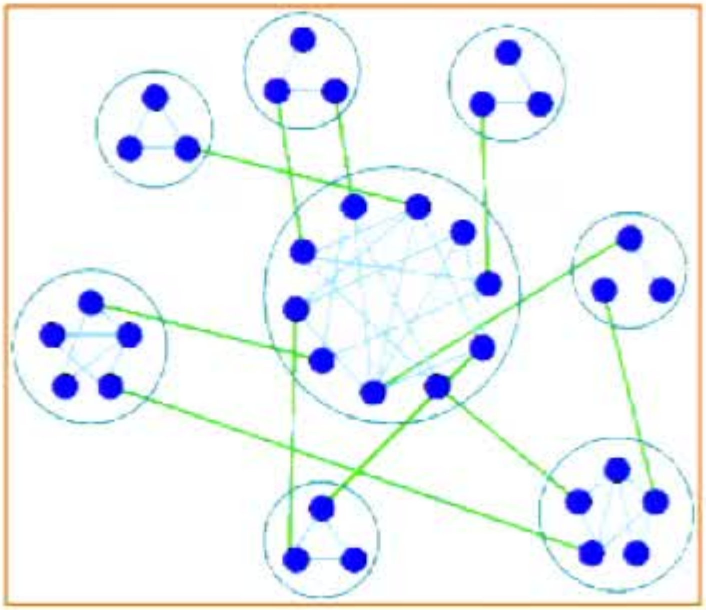
- Sparse direct factorization only viable for small problems
- Stationary iterations (Jacobi, Gauss-Seidel) converge but quite slowly
- Conjugate gradients or Chebyshev acceleration reduces #iterations.
  - Key is to find good preconditioner M≈A
- Classic "black-box" algebraic preconditioners:
  - Jacobi (diagonal)
  - Symmetric Gauss-Seidel (SGS)
  - Incomplete Cholesky (IC)
- Algebraic multigrid (AMG)
  - Developed for PDEs on meshes, not complex networks
  - Recent progress tuning for complex networks (LAMG)

BTER Graph Generator

How to generate realistic graphs/networks?

We use BTER: Block Two-level Erdös-Renyi

- Kolda, Pinar, Seshadri (2014)
- Captures skewed degree distributions
    - Not necessarily power-law
- Has community structure
- Able to "fit" real data
    - Degree distribution
    - Clustering coefficient



Experiments

- Study two groups of graphs
  - Real networks from UF and SNAP collections
    - Social networks, web graphs, collaboration networks, etc.
    - 25 graphs, up to 735K vertices (3.5M edges)
  - Synthetic graphs (BTER)
    - Log normal degree distribution, but vary sizes and avg. degree
- Solve singular Lx=b where the solution is a random vector, using projected PCG
  - Null-space is just the constant vector
  - Use Trilinos software (next slide)
- Solvers have two phases
  - Setup (preconditioner setup or symbolic+numeric factorization)
  - Solve (CG iteration or triangular solves)

Trilinos Computational Science Toolkit

- Collection of ~60 packages
  - Heroux et al., Sandia
- Trilinos Capabilities:
  - Scalable Linear & Eigen Solvers
  - Discretizations, Meshes & Load Balancing
  - Nonlinear & Optimization Solvers
  - Software Engineering Technologies & Integration
- Parallel:
  - MPI for distributed memory
  - Growing support for shared-memory (OpenMP, pthreads, CUDA)

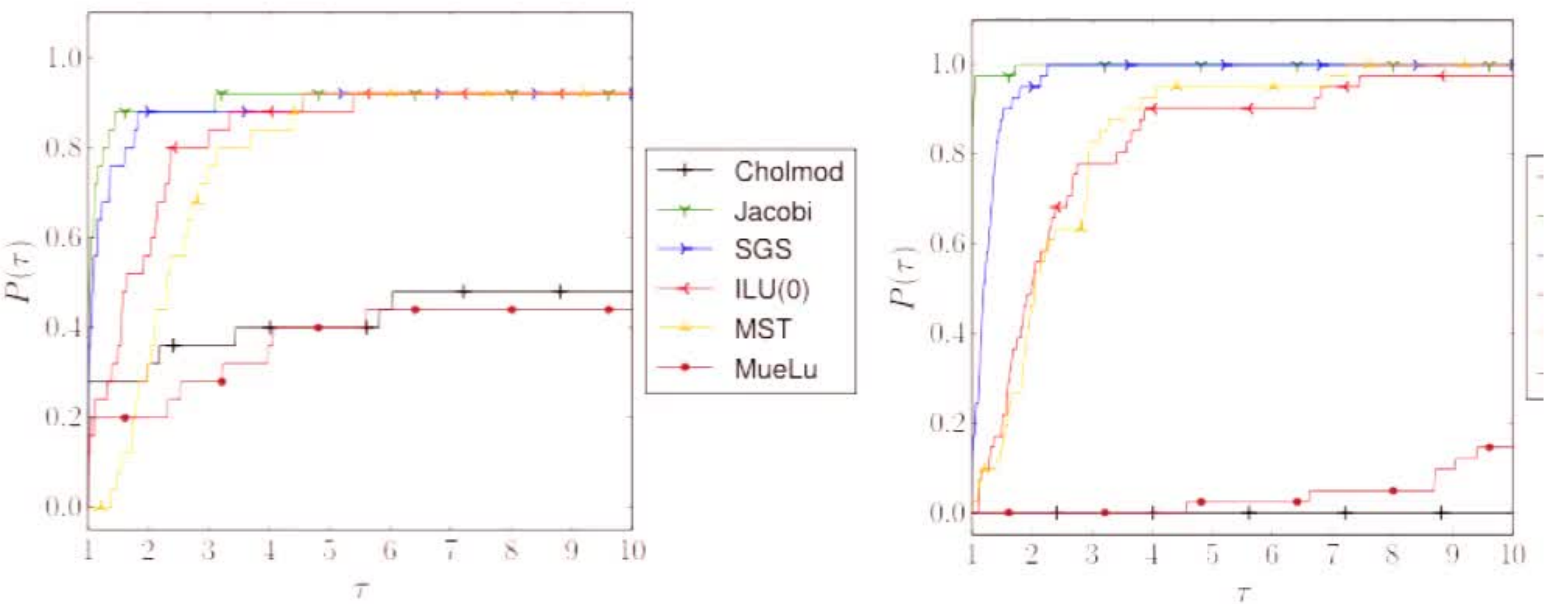
Packages we used:

- Tpetra: Matrices & vectors
- Belos: Iterative solvers
- Ifpack2: Preconditioners
  - Jacobi, Gauss-Seidel
  - Incomplete factorizations
  - Subgraph preconditioners
- MueLu: Multigrid

Performance Profile

Total time = Setup time + solve (iteration) time

- UF real networks
- BTER



Why do BTER differ from real graphs?

- BTER designed to match
  - Degree distribution
  - Clustering coefficient
  - Not eigenvalues!

- We tested BTER replica of Amazon-2008 network
  - Check #iterations for Laplacian solve

Graph	Cond.no.	Jacobi	SGS	ILU(0)	AMG
Original	1.5e5	3233	1290	1211	216
BTER	2.0e4	726	349	336	150

Combinatorial Preconditioners: Great in Theory

Core Idea: Construct a sparser graph that is a good spectral approximation (spectral sparsifier), use this as preconditioner.

- Typically, use a carefully chosen subgraph
  - For example, spanning tree + "a bit more"
- First proposed by Vaidya ('90, unpublished)
  - Described and analyzed in [Bern et al. '06], implemented by [Chen and Toledo, '03]
- Support theory extensions [B., Hendrickson, '03]
- A decade of improving complexity for Laplacian/SDD solvers
  - Significant work on "near optimal solvers"
    - Spielman & Teng ('04,'05), Koutis-Miller-Peng ('10,'11), others…
  - Kelner et al. ('13): dual randomized Kaczmarz
    - Lee & Sidford ('13): coordinate descent

Are They Competitive?

- Most combinatorial near-optimal solver/preconditioners are very complicated and have never been implemented
- The recent KOSZ/DRK method is simpler:
  - Solves a dual problem on the edges of the graph
  - Corresponds to flows in an electrical network
  - Randomly sample a cycle, update flow along edges, repeat
  - This is randomized Kaczmarz (on a dual problem)
  - No CG required as convergence is provably good without
- Two recent papers evaluate this method:
  - Hoske, Lukarski, Meyerhenke, Wegner (2015)
  - B., Deweese, Gilbert (2015)
  - Both conclude KOSZ/DRK is not competitive on unweighted graphs