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# Specialized System Solvers for very large Systems; Theory and Practice

### Gary Miller

Carnegie Mellon University join work with Yiannis Koutis, Richard Peng, Ali Sinop, and David Tolliver

Workshops on Algorithms for Modern Massive Data Sets June 18, 2010

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Outline						

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- 2 Symmetric Diagonally Dominate Systems
  - Graph Laplacians
- Applications of SDD/Laplacians
- Iterative Methods for Graph Laplacians
  - Combinatorial Preconditioners
- 5 Low Stretch Spanning Trees
- 6 Solver Code
  - Open Questions

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### Solving Linear Systems, a fundamental Problem

$$\begin{pmatrix} 3 & 2 & -1 \\ 2 & -5 & 4 \\ -1 & 1/2 & 2 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 3 \\ 7 \\ 2 \end{pmatrix}$$

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An Easy (	Case					

# • Upper and Lower Triangular Systems



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An Easy (	Case					

- Upper and Lower Triangular Systems
- O(m) time where m = number of nonzeros entries.

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An Easy (	Case					

- Upper and Lower Triangular Systems
- O(m) time where m = number of nonzeros entries.

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Goal: Find more easy cases that have applications.

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Symme	etric Matrio	ces and Po	ositive Defini	te		

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# • Assume A is symmetric, $A = A^{T}$ .

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### Symmetric Matrices and Positive Definite

- Assume A is symmetric,  $A = A^{T}$ .
- Assume A is positive definite,  $x^T A x > 0$  for  $x \neq 0$ .

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### Symmetric Matrices and Positive Definite

- Assume A is symmetric,  $A = A^{T}$ .
- Assume A is positive definite,  $x^T A x > 0$  for  $x \neq 0$ .
- Open: Can we solve spd systems in near linear time?

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### Symmetric Matrices and Positive Definite

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- Open: Can we solve spd systems in near linear time?

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 Two approaches to solving: direct and iterative methods.

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Direct Me Gaussian		on Matrices				

# Goal: algorithms that minimize work and space.

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Direct Mo Gaussia		on Matrice	s			

- Goal: algorithms that minimize work and space.
- Trick: View nonzero entries as an undirected graph and view pivoting as a graph operation.

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Good Pive	ot Strategi	es				

## 1970s and 1980s

Planar systems: O(n<sup>3/2</sup>) work and O(n log n) fill/space, [Lipton, Rose, Tarjan].

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Good P	ivot Strate	enies				

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Planar systems: O(n<sup>3/2</sup>) work and O(n log n) fill/space, [Lipton, Rose, Tarjan].

 3D Systems: O(n<sup>2</sup>) work and O(n<sup>3/2</sup>) fill/space, [M, Teng, Thurston, Vavasis] (EG: 3D images and 3D finite element).

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- 3D Systems: O(n<sup>2</sup>) work and O(n<sup>3/2</sup>) fill/space, [M, Teng, Thurston, Vavasis] (EG: 3D images and 3D finite element).
- *O*(*n*<sup>3/2</sup>) space is too big for 3D Image problems.

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Pure It	erative Me	thods				

Solving Ax = b. • Basic method:  $x^{(i+1)} = (I - A)x^{(i)} + b$ 





Solving Ax = b.

- Basic method:  $x^{(i+1)} = (I A)x^{(i)} + b$
- Convergence/Rate is determined by ||I A||.

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# Solving Ax = b.

- Basic method:  $x^{(i+1)} = (I A)x^{(i)} + b$
- Convergence/Rate is determined by ||I A||.
- Accelerated Methods: Chebyshev Iteration, Conjugate Gradient.

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Solving Ax = b.

• Basic method:  $x^{(i+1)} = (I - A)x^{(i)} + b$ 

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 Accelerated Methods: Chebyshev Iteration, Conjugate Gradient.

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• CG: *O*(*nm*), [ Magnus, Eduard 52 ].

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**Preconditioned Iterative Methods** 

Solving 
$$B^{-1}Ax = B^{-1}b$$
.

• Basic method:  $x^{(i+1)} = x^{(i)} + B^{-1}(b - Ax^{(i)})$ 

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### **Preconditioned Iterative Methods**

# Solving $B^{-1}Ax = B^{-1}b$ .

- Basic method:  $x^{(i+1)} = x^{(i)} + B^{-1}(b Ax^{(i)})$
- Computing x<sup>(i+1)</sup>
  - $r = b Ax^{(i)}$  Forward Multiply and addition.
  - Bz = r Solve the preconditioner system
     return x<sup>(i+1)</sup> = x<sup>(i)</sup> + z

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### **Preconditioned Iterative Methods**

# Solving $B^{-1}Ax = B^{-1}b$ .

- Basic method:  $x^{(i+1)} = x^{(i)} + B^{-1}(b Ax^{(i)})$
- Computing x<sup>(i+1)</sup>
  - $r = b Ax^{(i)}$  Forward Multiply and addition.
  - Bz = r Solve the preconditioner system
    return x<sup>(i+1)</sup> = x<sup>(i)</sup> + z
- Goal: Minimize the number of iteration while minimizing the cost of the solve.

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Classic	Preconditio	oners				

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# • Jacobi: B = Diagonal(A).

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Classic	Precondi	tioners				

- Jacobi: B = Diagonal(A).
- Gauss-Seidel: B = UpperTriangular(A).

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Classic	c Precondi	tioners				

- Jacobi: B = Diagonal(A).
- Gauss-Seidel: B = UpperTriangular(A).

• SSOR:  $B = (L + \frac{1}{\omega}D)\frac{1}{\omega}D(L + \frac{1}{\omega}D)$ 

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Classic	c Precondi	tioners				

- Jacobi: *B* = *Diagonal*(*A*).
- Gauss-Seidel: B = UpperTriangular(A).

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- SSOR:  $B = (L + \frac{1}{\omega}D)\frac{1}{\omega}D(L + \frac{1}{\omega}D)$
- Still too slow and unreliable.

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### • Def: A is SDD if:

$$orall i \quad oldsymbol{A}_{ii} \geq \sum_{j 
eq i} |oldsymbol{A}_{ij}|$$

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• Note: A is positive semi-definite.

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- Note: A is positive semi-definite.
- Subcase: SDD with nonpositive off diagonal Graph Laplacians

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$$orall i \quad {oldsymbol{A}}_{ii} \geq \sum_{j 
eq i} |{oldsymbol{A}}_{ij}|$$

• Note: A is positive semi-definite.

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- Subcase: SDD with nonpositive off diagonal Graph Laplacians
- SDD can be reduce to Graph Laplacians, [Gremban M 96]

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Graph Laplacians						
Graph La	placian					





Weighted incidence matrix:

$$m{A}_{ij} = \left\{egin{array}{cc} m{w}_{ij} & ext{if } m{e}_{ij} \in E \ 0 & ext{otherwise} \end{array}
ight.$$

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Weighted incidence matrix:

$$oldsymbol{A}_{ij} = \left\{egin{array}{cc} oldsymbol{w}_{ij} & ext{if } oldsymbol{e}_{ij} \in E \ 0 & ext{otherwise} \end{array}
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• Degree of 
$$v_i$$
:  $d_i = \sum_j w_{ij}$ 



Weighted incidence matrix:

$$oldsymbol{A}_{ij} = \left\{egin{array}{cc} oldsymbol{w}_{ij} & ext{if} egin{array}{c} oldsymbol{e}_{ij} \in E \ 0 & ext{otherwise} \end{array}
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• Degree of 
$$v_i$$
:  $d_i = \sum_j w_{ij}$   
•  $D = \begin{pmatrix} d_1 & 0 \\ & \ddots & \\ 0 & & d_n \end{pmatrix}$ 



Weighted incidence matrix:

$$A_{ij} = \left\{ egin{array}{cc} w_{ij} & ext{if } e_{ij} \in E \ 0 & ext{otherwise} \end{array} 
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• Degree of 
$$v_i$$
:  $d_i = \sum_j w_{ij}$ 

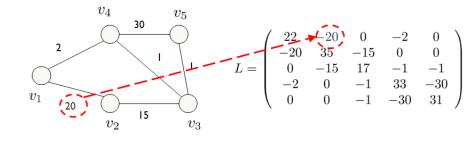
$$D=\left(egin{array}{ccc} d_1&&0\&\ddots&\&0&&d_n\end{array}
ight)$$

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• Laplacian: L = D - A

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Graph Laplacians						

### Example of Laplacian



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History for solving Laplacian								
Graph Laplacians								
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Recurrsive preconditioned iterative methods.

- $O(n^{1.2})$  for planar Laplacians, [Vaidya 91]
- $\tilde{O}(m^{1.5})$  for natural 3D graphs [Gremban, M 96].
- First near-linear time algorithm,  $O(m \log^{15} n)$ , [Spielman, Teng 04].
- O(n) for planar Laplacians, [Koutis, M 07]
- O(m log<sup>2</sup> n) (ignoring log log and lower terms), [Koutis, M, Peng 10].

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Graph Lapla	acians					
Main 1	Theorem					

#### Theorem

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[Koutis, M, Peng 10]

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### **Classic Applications of the Laplacian**

# • View each edge a conductor with conductance w<sub>ij</sub>.



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# **Classic Applications of the Laplacian**

• View each edge a conductor with conductance *w<sub>ij</sub>*.

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• Let V be a column vector of voltages

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# **Classic Applications of the Laplacian**

- View each edge a conductor with conductance  $w_{ij}$ .
- Let V be a column vector of voltages
- If *LV* = *c* then *c* is the residual current needed to maintain the given voltages.

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• View each edge as a conductor with conductance w<sub>ij</sub>.

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• View each edge as a conductor with conductance *w<sub>ij</sub>*.

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• Let *V* be a column vector of temperatures.

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- View each edge as a conductor with conductance *w<sub>ij</sub>*.
- Let V be a column vector of temperatures.
- If c = LV then c is the residual heat needed to maintain the given temperatures.

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Intro	SDD	Apps	Iterative	Trees	Code	Open

- View each edge as a conductor with conductance *w<sub>ij</sub>*.
- Let V be a column vector of temperatures.
- If c = LV then c is the residual heat needed to maintain the given temperatures.
- The finite element heat equations can be preconditioned with a graph Laplacian and thus solved in *O*(*n* + *m*) time. [Boman, Hendrickson, and Vavasis 06]

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Intro	SDD 0000	Apps	Iterative	Trees	Code	Open

#### Graph Laplacian's and Random Walks

Transition Matrix:  $A_G D^{-1}$ , symmetric *A*. Mixing Rate-Fundamental Eigenvector:  $\tilde{O}(n+m)$  [Spielman Teng 04] Trick: Inverse Powering only requires  $O(\log n)$  iterations.

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Laplacia	n's and Sp	ring Mass	Systems			

# • *G* = (*V*, *E*, *w*) weighted graph and *w*<sub>ij</sub> is viewed a spring constant.

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Laplaciar	n's and Spi	ring Mass s	Systems			

- *G* = (*V*, *E*, *w*) weighted graph and *w*<sub>ij</sub> is viewed a spring constant.
- M is a diagonal matrix of mass constants

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- *G* = (*V*, *E*, *w*) weighted graph and *w<sub>ij</sub>* is viewed a spring constant.
- M is a diagonal matrix of mass constants
- Fact: Modes of vibration of Spring-Mass system *G*, *M* are: Eigen-pairs of *L<sub>G</sub>x* = λ*Mx*.

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Lapla	cian's and S	Spring Ma	ss Systems			

- *G* = (*V*, *E*, *w*) weighted graph and *w*<sub>ij</sub> is viewed a spring constant.
- M is a diagonal matrix of mass constants
- Fact: Modes of vibration of Spring-Mass system *G*, *M* are: Eigen-pairs of  $L_G x = \lambda M x$ .
- Thus the fundamental mode can be found in  $\tilde{O}(n+m)$  time.

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Spring	Mass Sys	tem				

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Movie of a Simple Image

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Graph	Laplacian	's and Line	ar Programm	ning		

• Graph Maximum Flow Prob: Find a maximum flow from *s* to *t*.

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Graph Laplacian's and Linear Programming

- Graph Maximum Flow Prob: Find a maximum flow from *s* to *t*.
- Algorithm: Max-Flow is a LP problem so use log barrier interior point method.

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## Graph Laplacian's and Linear Programming

- Graph Maximum Flow Prob: Find a maximum flow from *s* to *t*.
- Algorithm: Max-Flow is a LP problem so use log barrier interior point method.
- Fact: Each of  $O(\sqrt{m})$  pivots requires the solution the graph Laplacian.

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# Graph Laplacian's and Linear Programming

- Graph Maximum Flow Prob: Find a maximum flow from *s* to *t*.
- Algorithm: Max-Flow is a LP problem so use log barrier interior point method.
- Fact: Each of  $O(\sqrt{m})$  pivots requires the solution the graph Laplacian.

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• Thus: Approximate Max-Flow is  $\tilde{O}((m+n)^{3/2})$ [Daitch, Spielman 08]

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Graph Laplacian's and Convex Programming

 Uniform TV Denoising: Input: image s
 Output: image arg min ||x − s||<sup>2</sup><sub>2</sub> + λ|| ∨ x||<sub>1</sub>

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#### Graph Laplacian's and Convex Programming

- Uniform TV Denoising: Input: image s
   Output: image arg min ||x − s||<sub>2</sub><sup>2</sup> + λ|| ∇ x||<sub>1</sub>
- Nonuniform TV Denoising: Input: pixel image s Output: arg min(x − s)<sup>T</sup>(x − s) + Sum<sub>(i,j)∈G</sub>|w<sub>ij</sub>(x<sub>i</sub> − x<sub>j</sub>)|

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### Graph Laplacian's and Convex Programming

- Uniform TV Denoising: Input: image s
   Output: image arg min ||x − s||<sub>2</sub><sup>2</sup> + λ|| ∇ x||<sub>1</sub>
- Nonuniform TV Denoising: Input: pixel image s Output: arg min(x − s)<sup>T</sup>(x − s) + Sum<sub>(i,j)∈G</sub>|w<sub>ij</sub>(x<sub>i</sub> − x<sub>j</sub>)|

• Use log-barrier interior point: pivots are low rank perturbation of Laplacian, Thus:  $\tilde{O}((m+n)^{3/2})$  time. [Koutis M Peng Sinop Tolliver 09]

Intro	SDD 0000	Apps	Iterative •oooooooooo	Trees 0000	Code	Open
Combinatoria	al Preconditioners					
Condit	ion Numbe	er				

- **Def:**Condition number of *A* and *B*,  $\kappa(B^{-1}A) = \lambda_{max}(B^{-1}A)/\lambda_{min}(B^{-1}A).$
- OR: If  $x^T A x \le x^T B x \le k x^T A x$  for all  $x \in \mathbb{R}^n$ , then  $\kappa(B^{-1}A) \le k$

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Combinatori	al Preconditioners					
Rate o	of Converge	ence				

- Classical results, measured in number of iterations per bit of precision.
- Richardson iteration:  $O(\kappa(B^{-1}A))$ , too slow.
- Conjugate gradient: O(√κ(B<sup>-1</sup>A)) or better, hard to analyze when B is called recursively and solved inexactly.

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• Chebyshev iteration:  $O(\sqrt{\kappa(B^{-1}A)})$ , will use.

When	When is B a Good Recursive Preconditioner?									
Combinatori	al Preconditioners									
Intro	SDD 0000	Apps	Iterative oo●ooooooo	Trees	Code	Open				

- Properties that Laplacian *B* should have:
  - **1**  $B^{-1}A$  has low condition number.
  - Quickly reduces to something that can be solved faster (smaller size).
- Examples:
  - [Vaidya 91] Spanning tree + a few edges.
  - [Gremban, M 96] Steiner tree.
  - [Boman, Hendrickson 03; Spielman, Teng 04] Low stretch spanning tree + a few edges.
  - [Koutis, M 07] Partition planar graphs into pieces of size k with  $\sqrt{k}$  boundary, optimally precondition each piece.

Intro	SDD 0000	Apps	Iterative ○○○●○○○○○○○	Trees 0000	Code	Open			
Combinatorial Preconditioners									
Getting	Getting a Good Preconditioner.								

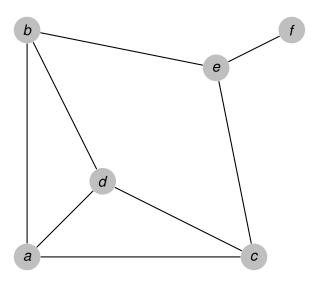
Main steps:

- Find a sparse subgraph by random sampling.
- Use Gaussian elimination to remove degree 1 and 2 vertices.
- We need sampling to be fast and give good condition numbers.

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Combinatorial P	reconditioners					

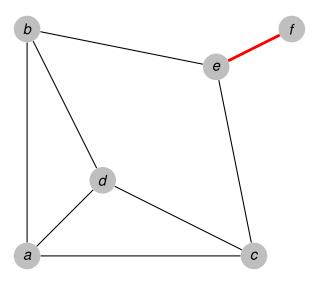
# Example: Pivoting out degree 1 and 2.



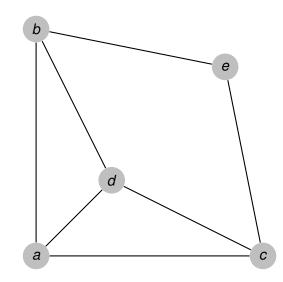
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Combinatorial Prec	onditioners					

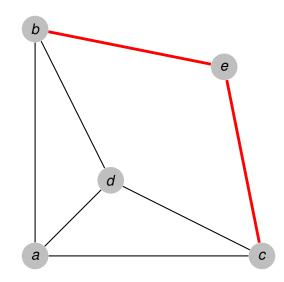
# Example: Pivoting out degree 1 and 2.



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Combinator	al Preconditioners					
Pivot(	f)					



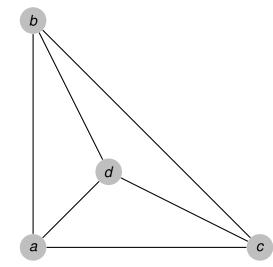
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Combinatori	ial Preconditioners					
Pivot(	f)					



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Combinator	ial Preconditioners					
Pivot(	e)					

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Ran out of degree 1 or 2 nodes, quit.



Given a graph G find H by: Remove most edges, increase weight of remaining edges.

Possible properties to be preserved:

- Spanners: distance, diameter
- Cut sparsifier: weight of cut for all 2<sup>|V|</sup> subset of vertices
- Triangle sparsifiers: number of triangles in a subgraph
- We want spectral sparsifiers
- Also want *H* to be ultra-sparse for Gaussian elimination to make progress.

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 Need to reduce to n - 1 + m/c edges for in order to decrease edge count by factor of c/3.

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Combinatorial Preconditioners								
Previo	Previous Work on Sparsification							

- Expanders: sparsifier for complete graph.
- Ramanujan graphs: optimal spectral sparsifiers for the complete graph.
- [Benczur, Karger 96] Cut sparsifiers,  $O(n \log n)$  edges.
- [Kolountzakis, M, Tsourakakis 10] Edge sampling can give good triangle sparsifiers.

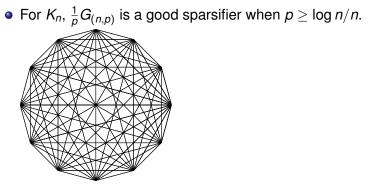
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Previous Work on Spectral Sparsification								
Combinatori	al Preconditioners							
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- [Spielman, Teng 04] H has Õ(n) edges, constant condition number.
- [Spielman, Teng 04] Ultrasparsifier, *H* has n 1 + n/c edges, condition number  $\tilde{O}(c)$ .
- [Spielman, Srivastava 08] Conceptually simple sampling algorithm for spectral sparsification.
- [Batson, Spielman, Srivastava 09] and [Kolla, Makarychev, Saberi, Teng 10] gave better bounds, but their algorithms do not run in near-linear time.

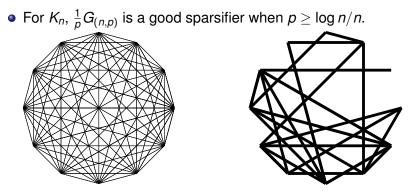
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Combinatoria	al Preconditioners							
Sparsi	Sparsifier for the Complete Graph							



 Sidenote: examples generated by code in the TeX file, different sparsifier every time slides are generated.





 Sidenote: examples generated by code in the TeX file, different sparsifier every time slides are generated.

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Combinatori	al Preconditioners									
Gener	Generalized Graph Sampling									

• [Benczur, Karger 96] used this method for cut sparsifiers

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- Near-linear time spectral sparsifiers use the same framework.
- Compute a probability *p<sub>e</sub>* for each edge.
- For each edge *e* keep with probability *p<sub>e</sub>*.
   If kept multiply weight by 1/*p<sub>e</sub>*.

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Combinatorial Preconditioners										
What S	Sampling C	aives								

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- Expected value: original graph
- Expected number of edges:  $(\sum_e p_e) \log n$ .
- Concentration?

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Combinatoria	al Preconditioners					
Effecti	ve Resista	nce				

- Consider each edge as a resistor with conductance w<sub>e</sub>
- For edge e = (u, v) let  $R_e$  be the effective resistance from u to v in G.

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Sparsi	fication by	Effective	Resistance			
Combinatori	al Preconditioners					
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#### Theorem (Spielman, Srivastava 08)

Sampling a weighted graph G using edge probablities  $p_e = w_e R_e$  to generate H with  $O(n \log n)$  expected edges then  $\kappa(G, H)$  is a constant with high probablity.

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#### Calculating effective resistance efficiently?

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Low S	Stretch Span	ning Trees	s			

We use low stretch spanning trees to approximate effective resistance.

Let T be a tree of G

#### Definition

Stretch(e) =  $w_e \cdot ER_e^T$ , the effective resistance in *T*.

$$stretch(T) = \sum_{e \in G} stretch(e)$$

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Low Stretch Spanning Trees

- [Spielman, Teng 04] Fundamental for their solver and ultrasparsifier.
- [Kolla, Makarychev, Saberi, Teng 10] Fundamental their near-optimal sparsifier.

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#### Known Results about Low Stretch Spanning Trees

 First studied in [ Alon, Karp, Peleg, West 95 ] in the context of k server problem.

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- [Elkin, Emek, Spielman, Teng 05]  $O(m \log^2 n)$  stretch.
- [Abraham, Bartal & Neiman 08] roughly  $O(m \log n)$  stretch.

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#### Example of Low Stretch Spanning Tree on a Unit Weight Mesh

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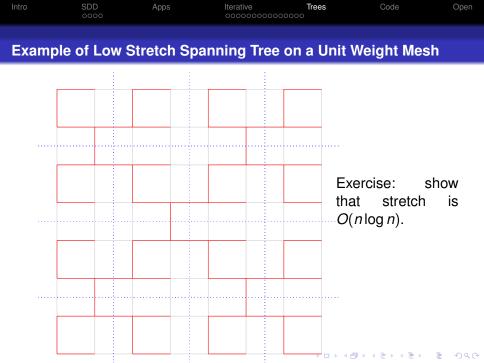
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#### Example of Low Stretch Spanning Tree on a Unit Weight Mesh



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Pseud	ocode					

INCREMENTAL SPARSIFY Input: Graph *G*, real value  $c = O(log^4 n)$ . Output: Graph *H* that's a sparsifier for *G* 

- $T \leftarrow \text{LowStretchTree}(G)$
- Let T' be T scaled up by factor of c
- 3 Let G' be the graph obtained from G by replacing T with T'

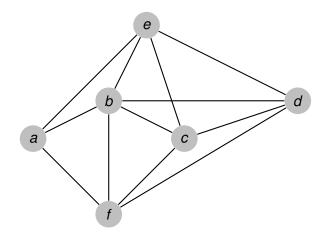
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- ④ FOR  $oldsymbol{e}\in oldsymbol{E}$
- Solution Calculate EffectiveResistance<sub>T'</sub>(e)</sub>
- 6 ENDFOR
- $H \leftarrow \mathsf{SAMPLE}(G', EffectiveResistance_{T'})$
- 🖲 return H

Intro	SDD 0000	Apps	Iterative	Trees o	Code	Open

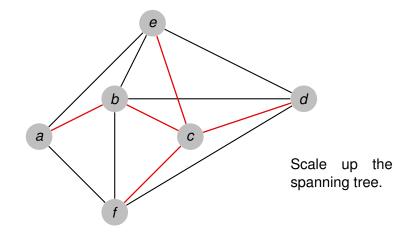
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#### **Example: Original Graph**



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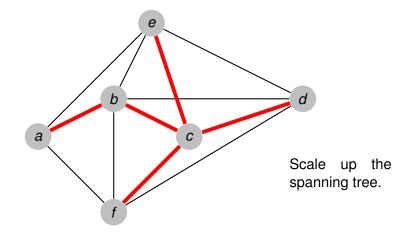
#### Example: Scale up a Good Spanning Tree



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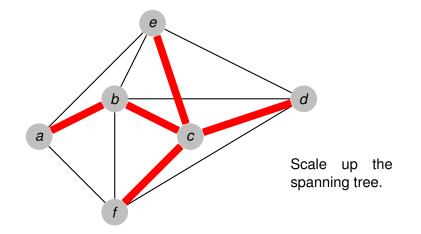
#### Example: Scale up a Good Spanning Tree



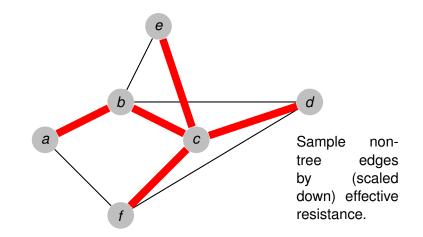
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#### Example: Scale up a Good Spanning Tree

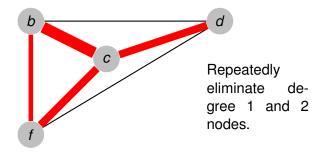


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Example	: Sample					



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#### **Example: Gaussian Elimination**



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### • 1950's $O(n^2)$ (Conjugate Gradient)

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## 1950's O(n<sup>2</sup>) (Conjugate Gradient)

• 1970's  $O(n^{1.5})$  (Nested Dissection) (LRT)

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- 1950's  $O(n^2)$  (Conjugate Gradient)
- 1970's  $O(n^{1.5})$  (Nested Dissection) (LRT)

 1990's O(n<sup>1.2</sup>) (Combinatorial Preconditioners) (Vaidya)



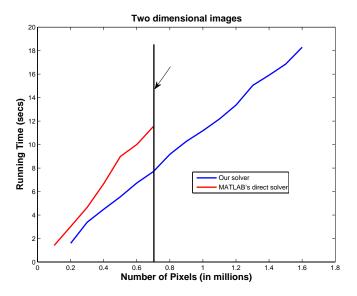
- 1950's  $O(n^2)$  (Conjugate Gradient)
- 1970's  $O(n^{1.5})$  (Nested Dissection) (LRT)
- 1990's O(n<sup>1.2</sup>) (Combinatorial Preconditioners) (Vaidya)
- 2000's O(n log<sup>2</sup> n) (Low stretch spanning trees) (ST)



- 1950's  $O(n^2)$  (Conjugate Gradient)
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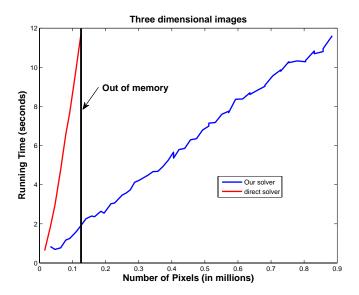
2006's O(n) (separator based preconditioners) (KM)





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Open (	Questions					

- Find fast methods for any SPD system.
- Find spectral methods that find better cuts by using more than one eigenvector.
- Find solvers that work in the L<sub>2</sub> norm.
- A implementable solver with near linear time guarantees. The low stretch spanning tree is the bottleneck!

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# Thank You