Approximate Gaussian Elimination and Applications

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UToronto

Laplacian Paradigm 2.0

FOCS 2018

Gaussian Elimination

Gaussian Elimination

$$
\begin{array}{rrrrcr}
16x_1 & -4x_2 & -8x_3 & -4x_4 & = & 16 \\
-4x_1 & +5x_2 & & -x_4 & = & -6 \\
-8x_1 & & +9x_3 & -x_4 & = & -19 \\
-4x_1 & -x_2 & -x_3 & +7x_4 & = & 11
\end{array}
$$

Gaussian Elimination

Add $^1/_4$ x Eq. 1 to Eq. 2

$$
\begin{array}{rrrrcr}
16x_1 & -4x_2 & -8x_3 & -4x_4 & = & 16 \\
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\end{array}
$$

Gaussian Elimination

Eliminated the first variable

$$
\begin{array}{rrrrr}
16x_1 & -4x_2 & -8x_3 & -4x_4 & = & 16 \\
 & +4x_2 & -2x_3 & -2x_4 & = & -2 \\
 & -2x_2 & +5x_3 & -3x_4 & = & -11 \\
 & -2x_2 & -3x_3 & +6x_4 & = & 15
\end{array}
$$

Gaussian Elimination

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\begin{array}{rrrrcr}
16x_1 & -4x_2 & -8x_3 & -4x_4 & = & 16 \\
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Gaussian Elimination

Consider the coefficient matrix

$$\begin{array}{rrrrcr} 16x_1 & -4x_2 & -8x_3 & -4x_4 & = & 16 \\ -4x_1 & +5x_2 & & -x_4 & = & -6 \\ -8x_1 & & +9x_3 & -x_4 & = & -19 \\ -4x_1 & -x_2 & -x_3 & +7x_4 & = & 11 \end{array}$$

$$\begin{bmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 9 & -1 \\ -4 & -1 & -1 & 7 \end{bmatrix}$$

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Symmetric

Gaussian Elimination

$$\begin{bmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 9 & -1 \\ -4 & -1 & -1 & 7 \end{bmatrix} = \begin{bmatrix} 1 \\ -\frac{1}{4} \\ -\frac{1}{2} \\ -\frac{1}{4} \end{bmatrix} \begin{bmatrix} 16 & -4 & -8 & -4 \end{bmatrix} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 4 & -2 & -2 \\ 0 & -2 & 5 & -3 \\ 0 & -2 & -3 & 6 \end{bmatrix}$$

Symmetric

Symmetric rank 1

Cholesky Factorization

$$\begin{bmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 9 & -1 \\ -4 & -1 & -1 & 7 \end{bmatrix} = \begin{bmatrix} 4 \\ -1 \\ -2 \\ -1 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ -2 \\ -1 \end{bmatrix}^{\mathsf{T}} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 4 & -2 & -2 \\ 0 & -2 & 5 & -3 \\ 0 & -2 & -3 & 6 \end{bmatrix}$$

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Symmetric

Symmetric rank 1

Schur Complement

Cholesky Factorization

$$\begin{bmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 9 & -1 \\ -4 & -1 & -1 & 7 \end{bmatrix} = \begin{bmatrix} 4 \\ -1 \\ -2 \\ -1 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ -2 \\ -1 \end{bmatrix}^{\mathsf{T}}$$

PSD

$$+ \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 4 & -2 & -2 \\ 0 & -2 & 5 & -3 \\ 0 & -2 & -3 & 6 \end{bmatrix}$$

The Schur complement is PSD.

Cholesky Factorization

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Cholesky Factorization

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$$= \begin{bmatrix} 4 & -1 & -2 & -1 \\ 0 & 2 & -1 & -1 \\ 0 & 0 & 2 & -2 \\ 0 & 0 & 0 & 1 \end{bmatrix}^{\mathsf{T}} \begin{bmatrix} 4 & -1 & -2 & -1 \\ 0 & 2 & -1 & -1 \\ 0 & 0 & 2 & -2 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$= U^{\mathsf{T}}U$ $\quad$ U is upper triangular

Solving $Lx = b$

Cholesky Factorization

Find U, upper triangular matrix, s.t.

$$U^\top U = L$$

Then solve

$$x = L^{-1}b = U^{-1}U^{-\top}b$$

Both inverses easy to apply!

Cholesky Factorization on Laplacians

$$L = \begin{bmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 9 & -1 \\ -4 & -1 & -1 & 6 \end{bmatrix}$$

$$= \begin{bmatrix} 4 \\ -1 \\ -2 \\ -1 \end{bmatrix} \begin{bmatrix} 4 \\ -1 \\ -2 \\ -1 \end{bmatrix}^{\mathsf{T}} + \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 4 & -2 & -2 \\ 0 & -2 & 5 & -3 \\ 0 & -2 & -3 & 5 \end{bmatrix}$$

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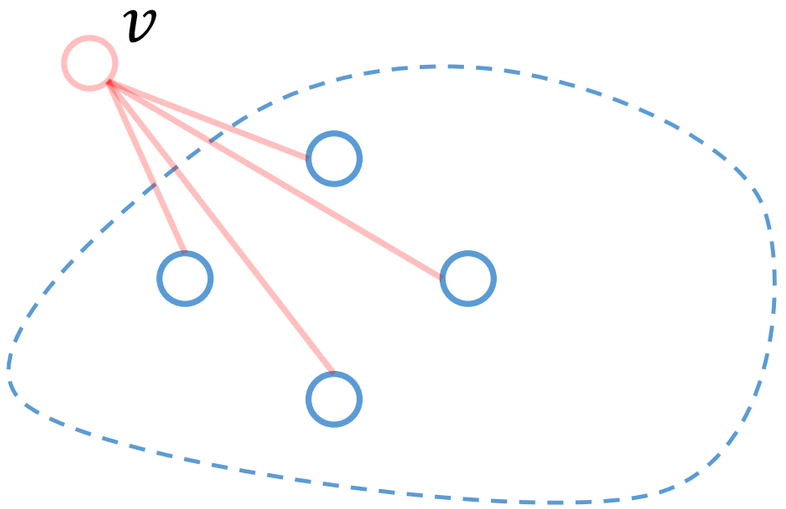
Another Laplacian!

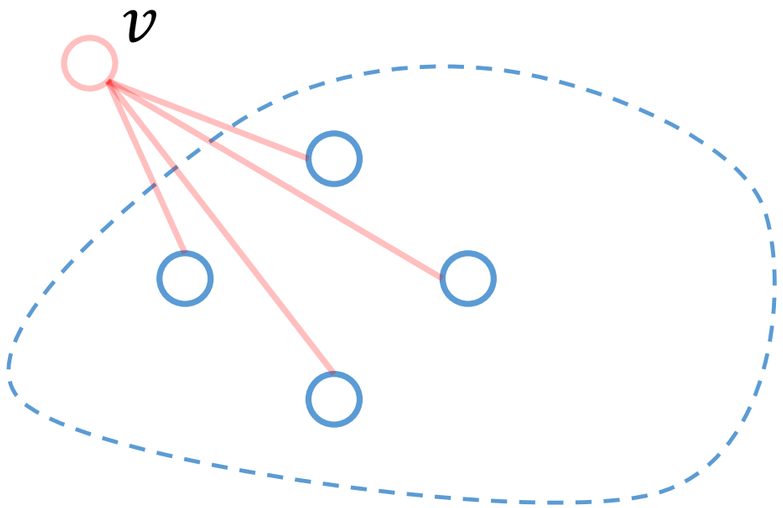
Cholesky Factorization on Laplacians

$L =$

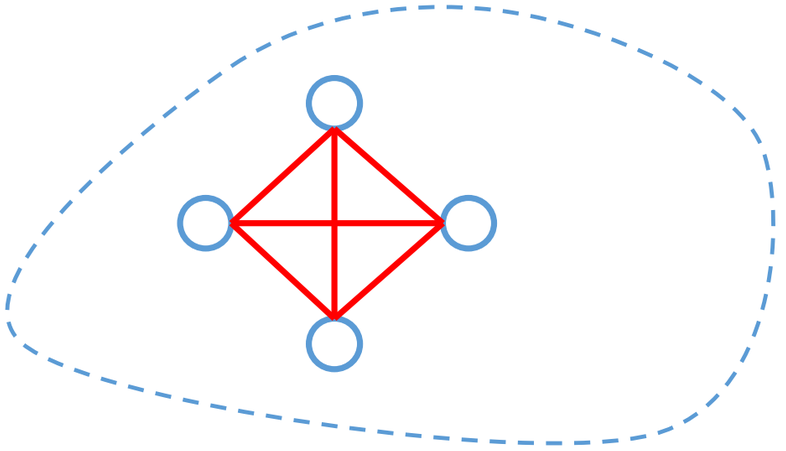


Cholesky Factorization on Laplacians

$L =$



Schur complement $=$



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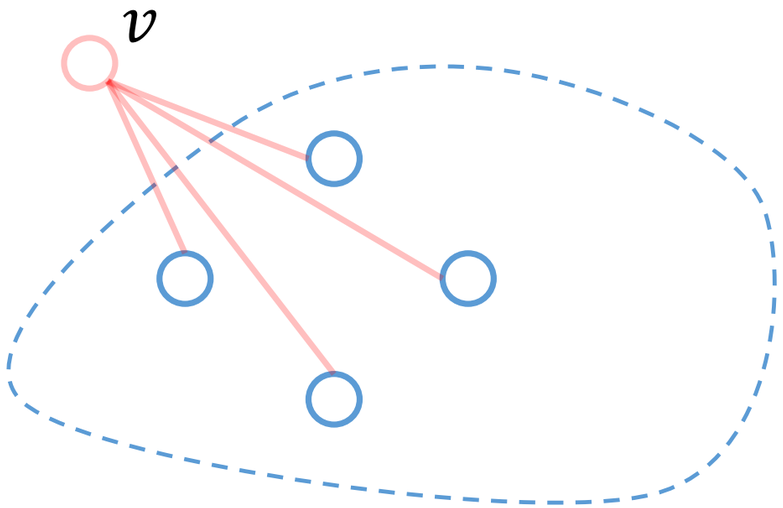

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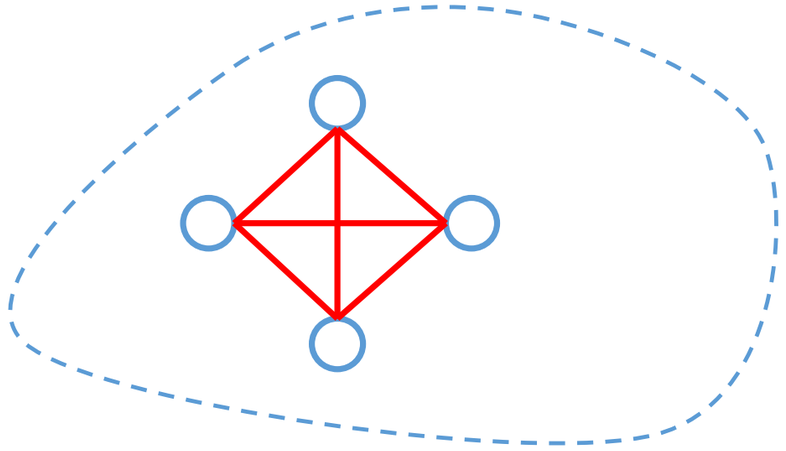
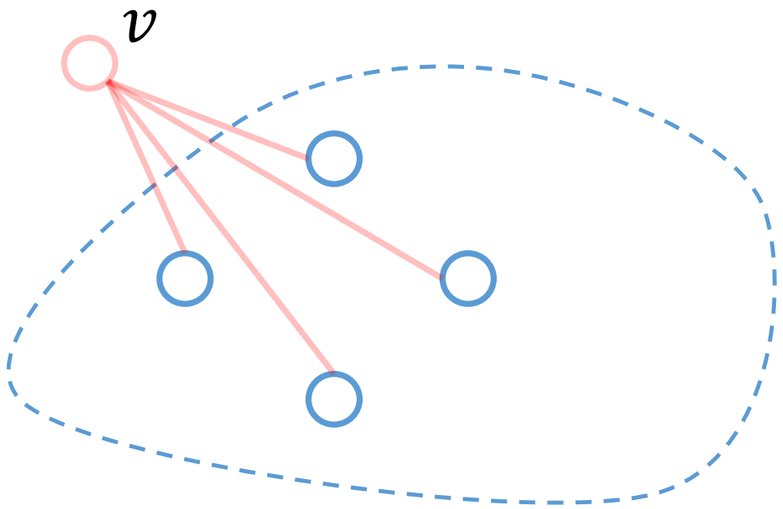


Elimination creates a clique on the neighbors of v

Cholesky Factorization on Laplacians

1. Pick a vertex v to eliminate
2. Add the clique created by eliminating v
3. Repeat

$L =$



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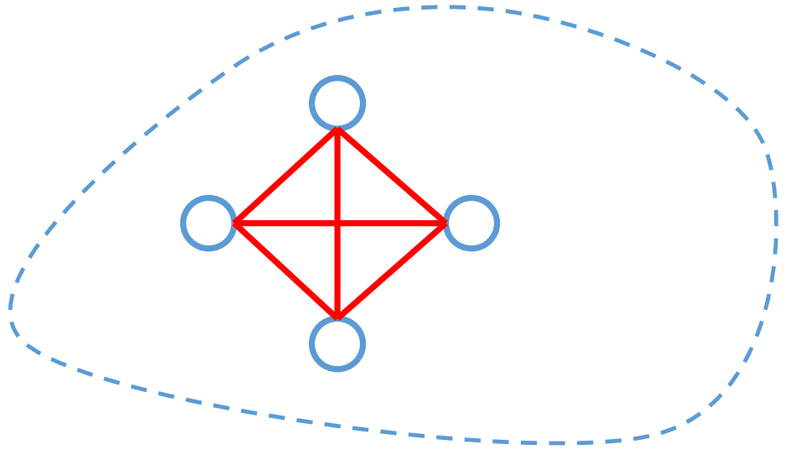
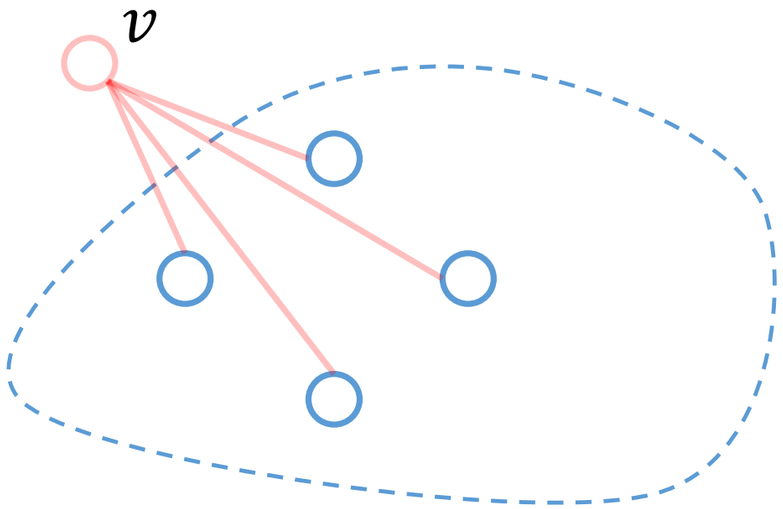


Elimination creates a clique on the neighbors of v

Why is Cholesky Factorization Slow?

$L =$



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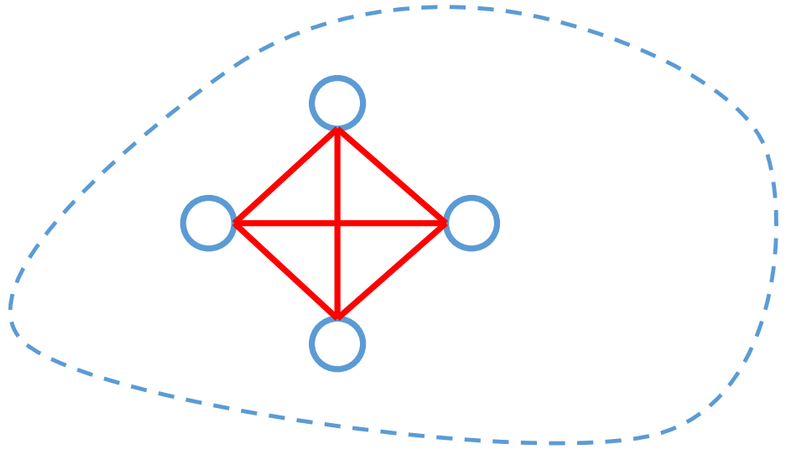

Elimination creates a clique on the neighbors of v

Why is Cholesky Factorization Slow?

The main issue is **fill.** Remove $\deg(v)$ edges, insert $\sim\deg(v)^2$ edges.

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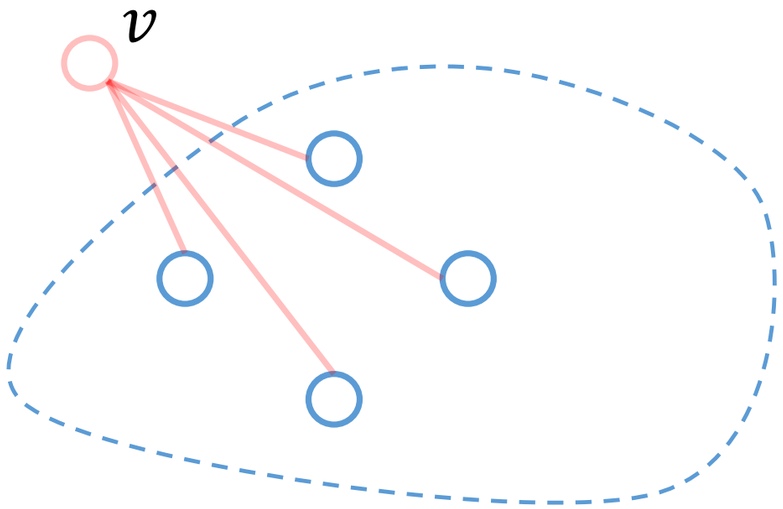

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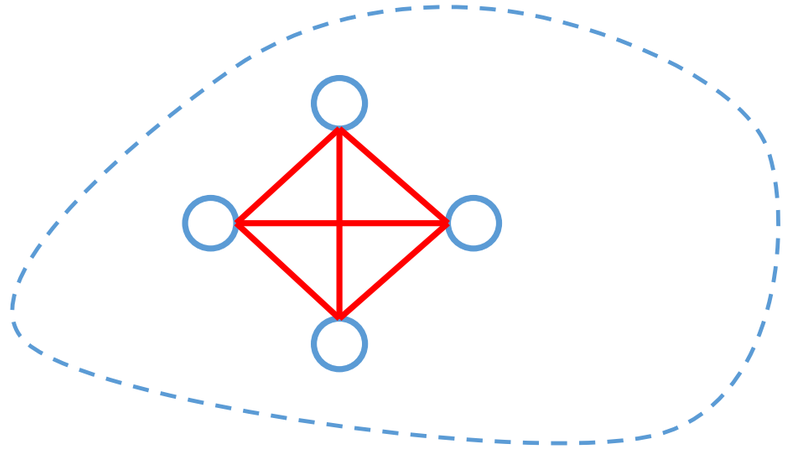

Elimination creates a clique on the neighbors of v

Why is Cholesky Factorization Slow?

Eliminate n vertices $\times$ add clique:

$$O\left(\sum_{v} \deg(v)^2\right) = O(n^3)$$

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Central challenge in scientific computing. Numerous heuristic approaches to sparse Cholesky factorization, back to [Varga '60]

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None provide guarantees for general Laplacians.

One-by-one Laplacian solver

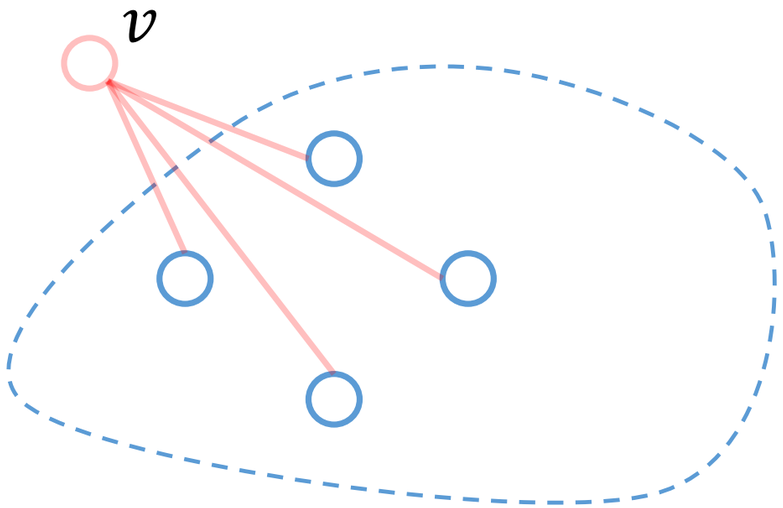
Fast Approximate Cholesky Factorization [Kyng-S ‘16]

Building on [Lee-Peng-Spielman ‘15]

Inspiration for the Paper

Elimination creates a clique on the neighbors of v

$L =$



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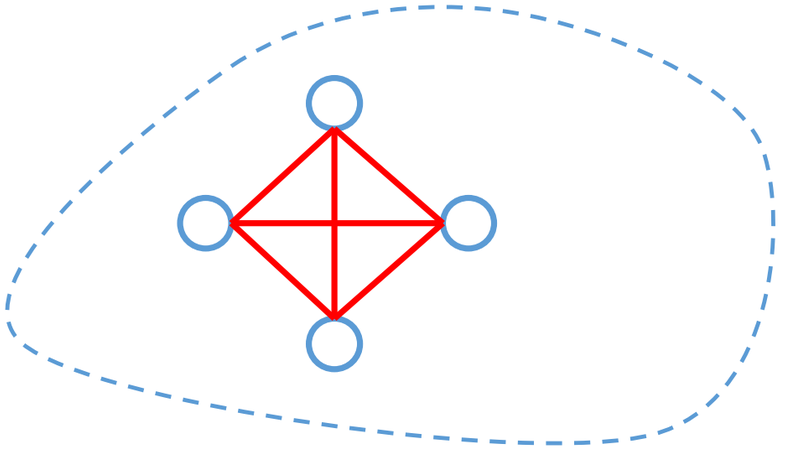

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Elimination creates a clique on the neighbors of v

Cliques can be sparsified!

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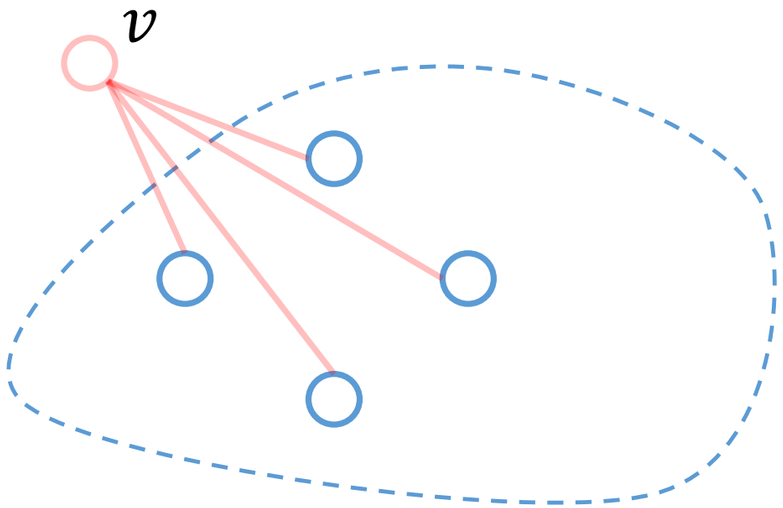

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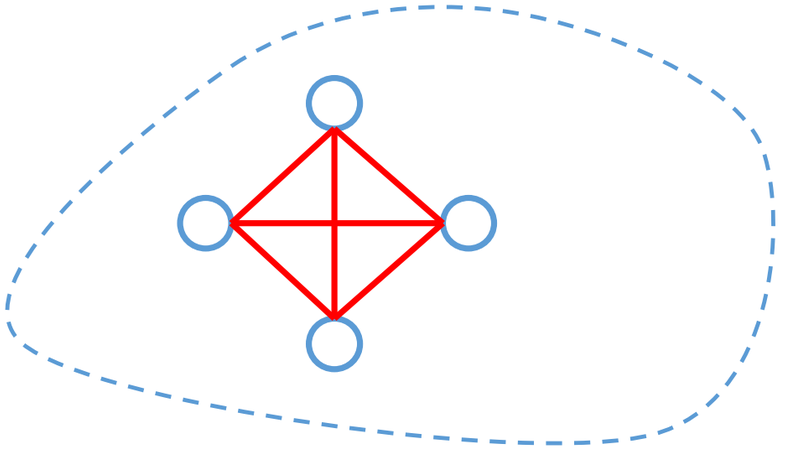

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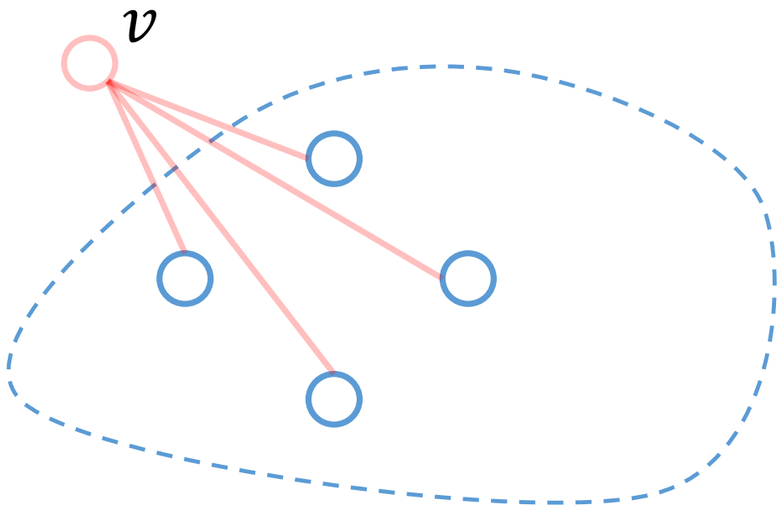
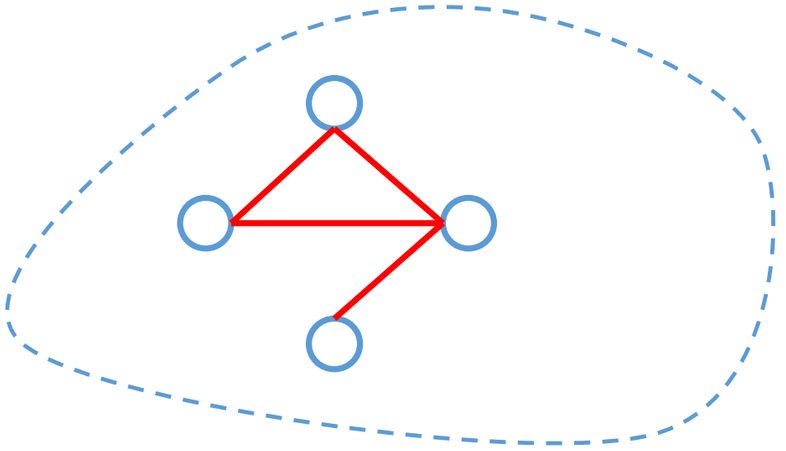


Schur complement $\approx_\delta$

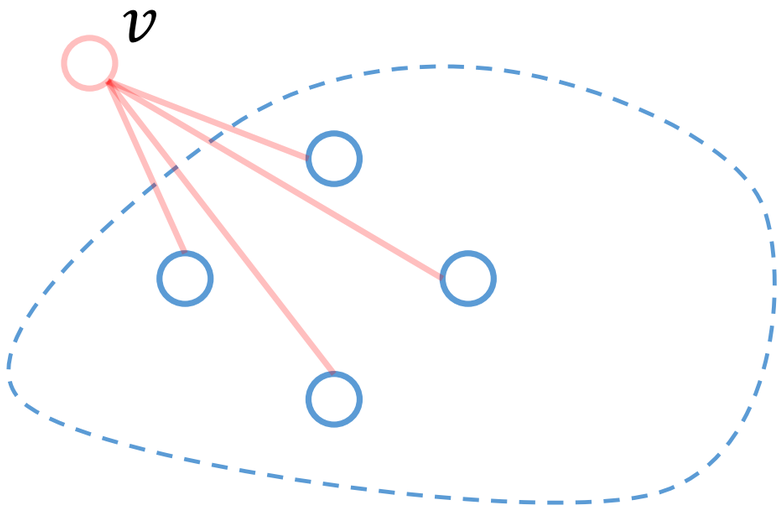


Inspiration for the Paper

Elimination creates a clique on the neighbors of v

Cliques can be sparsified! Replacing with an expander not enough.

$L =$



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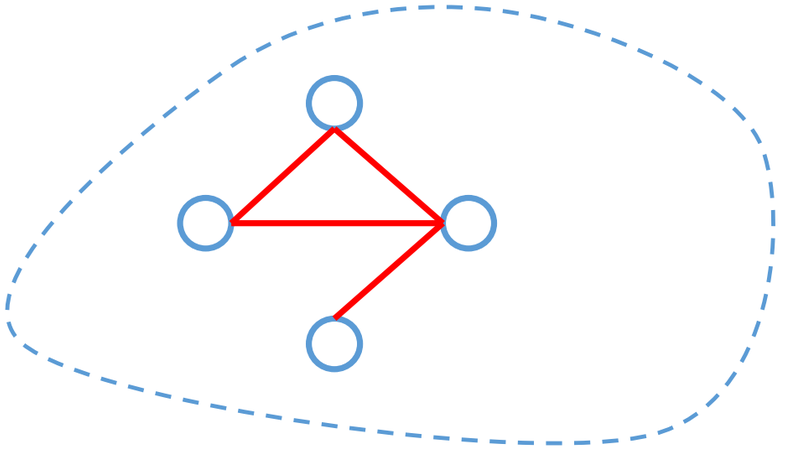

Sparse Cholesky Factorization

[Kyng-S'17]

1. Pick a random vertex v to eliminate
2. Sample $\deg(v)$ edges from the clique created by eliminating v
3. Repeat

Sparse Cholesky Factorization

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1. Pick a random vertex v to eliminate
2. Sample $\deg(v)$ edges from the clique created by eliminating v
3. Repeat

Most heuristic algorithms have a similar flavor.

e.g. Incomplete Cholesky Factorization (ICC)

Key difference: which edges to keep

What makes [Kyng-S'17] work?

First provably approximate sparse Cholesky factorization we're aware of

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What makes [Kyng-S'17] work?

First provably approximate sparse Cholesky factorization we're aware of

1. Maintains a PSD matrix as approximation with same kernel as L
2. At each step, correct expectation: $\mathbb{E}\, U^\top U = L$. Analysis using matrix martingales
3. Number of edges in remaining graph does not increase

Running Time

[Kyng-S'17] **Sparsified Cholesky Factorization**

Eliminate n vertices $\times$ add sparsified clique:

$$\tilde{O}\left(\sum_{v} \deg(v)\right) = \tilde{O}(m)$$

Sparse, Approximate Cholesky Factorization

[Kyng-S ‘16] For any Laplacian L, in time $O(m \log^3 n)$, can compute an upper triangular U s.t.

$$U^\top U \approx_{0.1} L$$

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Approximate Schur Complements

[Kyng-S ’16, Durfee-Kyng-Peebles-Rao-S ’17, Kyng ‘17]

Cholesky Factorization : Another view

$$L = \left[\begin{array}{c|c} a & b^{\mathsf{T}} \\ \hline b & C \end{array}\right] = \frac{1}{a}\begin{bmatrix} a \\ b \end{bmatrix}\begin{bmatrix} a \\ b \end{bmatrix}^{\mathsf{T}} + \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & C - \frac{1}{a}bb^{\mathsf{T}} \end{array}\right]$$

Rank 1

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Schur complement

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$$L = \left[\begin{array}{c|c} a & b^{\top} \\ \hline b & C \end{array}\right] = \frac{1}{a}\begin{bmatrix} a \\ \hline b \end{bmatrix}\begin{bmatrix} a \\ \hline b \end{bmatrix}^{\top} + \begin{array}{c} \begin{matrix} \bar{F} & F \end{matrix} \\ \left[\begin{array}{c|c} 0 & 0 \\ \hline 0 & C - \frac{1}{a}bb^{\top} \end{array}\right] \end{array} \begin{matrix} \\ \bar{F} \\ F \end{matrix}$$

Schur complement $Sc(L, F)$

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Schur complement $Sc(L, F)$

$$= \left[\begin{array}{c|c} 1 & 0 \\ \hline \frac{1}{a}b & I \end{array}\right]\left[\begin{array}{c|c} a & 0 \\ \hline 0 & C - \frac{1}{a}bb^{\mathsf{T}} \end{array}\right]\left[\begin{array}{c|c} 1 & \frac{1}{a}b^{\mathsf{T}} \\ \hline 0 & I \end{array}\right]$$

Partial Cholesky Factorization

Can eliminate several vertices at once. The order is irrelevant.

$$L = \begin{array}{c} \\ \bar{F} \\ F \end{array} \overset{\begin{array}{cc} \bar{F} & F \end{array}}{\left[\begin{array}{c|c} A & B^{\mathsf{T}} \\ \hline B & C \end{array}\right]}$$

$$= \begin{bmatrix} I & 0 \\ \hline BA^{-1} & I \end{bmatrix} \begin{bmatrix} A & 0 \\ \hline 0 & C - BA^{-1}B^{\mathsf{T}} \end{bmatrix} \begin{bmatrix} I & A^{-1}B^{\mathsf{T}} \\ \hline 0 & I \end{bmatrix}$$

Approximate Schur Complement

[Kyng-S ’16]

For any Laplacian L, any set F, in time $O(m\varepsilon^{-2}\log^3 n)$, can compute a graph H on F such that

$$L_H \approx_\varepsilon Sc(L,F)$$

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Applications of Approximate Schur Complement

1. Faster estimation of effective resistances + Sample Random Spanning trees
   [Durfee-Kyng-Peebles-Rao-S ’17, Durfee-Peebles-Peng-Rao ’17]

   Schur complements preserve effective resistances

Applications of Approximate Schur Complement

1. Faster estimation of effective resistances + Sample Random Spanning trees
   [Durfee-Kyng-Peebles-Rao-S ’17, Durfee-Peebles-Peng-Rao ’17]

2. Estimate Determinants of Laplacians / number of spanning trees
   [Durfee-Peebles-Peng-Rao ’17]

Spectral Sketches for Schur Complement

[Chu-Gao-Peng-S-Sawlani-Wang ’18 (this FOCS)]
Spectral sketch of Schur complement (weaker than spectral approximation)
Better ε dependence, worse $n^{o(1)}$ factors, in size / running time

Builds on [Andoni-Chen-Krauthgamer-Qin-Woodruff-Zhang ‘16, Jambulapati-Sidford ‘18].

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Faster estimation of Laplacian determinant.

Recursive solver for Connection Laplacians

[Kyng-Lee-Peng-S-Spielman ‘16]

Exact solvers via Partial Cholesky Factorization

$$L = \left[\begin{array}{c|c} I & 0 \\ \hline BA^{-1} & I \end{array}\right] \left[\begin{array}{c|c} A & 0 \\ \hline 0 & S \end{array}\right] \left[\begin{array}{c|c} I & A^{-1}B^{\top} \\ \hline 0 & I \end{array}\right]$$

$$S = C - BA^{-1}B^{\top}$$

Schur complement $Sc(L, F)$

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Compute L^{-1} = Compute A^{-1} + Compute S^{-1} + $O(1)$ multiplications

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Exact solvers via Partial Cholesky Factorization

Compute L^{-1} = Compute A^{-1} + Compute S^{-1} + $O(1)$ multiplications

$$T(n) = 2T(n/2) + O(n^{\omega})$$
$$= O(n^{\omega})$$

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Fast solvers via Partial Cholesky Factorization?

Find a submatrix A such that S can be efficiently approximated,

And recurse on A, S?

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Need a family of matrices closed under Schur complements

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Laplacians, Connection Laplacians

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Laplacians

Connection Laplacians

Laplacians

$n \times n$ matrix

Every vertex $\mathrm{x_u} \in \mathbb{R}$

Connection Laplacians

$kn \times kn$ matrix (k fixed, say 3)

Every vertex $\mathrm{y_v} \in \mathbb{C}^k$

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$U_{u,v}$ is unitary

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Applications in cryo-em, image alignment

Fast solvers for Connection Laplacians

Find a submatrix A such that S can be efficiently approximated,

$$S = C - BA^{-1}B^{\top}$$

Schur complement

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Fast solvers for Connection Laplacians

Find a submatrix A such that S can be efficiently approximated,

"strongly diagonally dominant sets"

$$S = C - BA^{-1}B^{\top}$$

Schur complement

$$L^{-1} = \begin{bmatrix} I & -A^{-1}B^{\top} \\ 0 & I \end{bmatrix} \begin{bmatrix} A^{-1} & 0 \\ 0 & S^{-1} \end{bmatrix} \begin{bmatrix} I & 0 \\ -BA^{-1} & I \end{bmatrix}$$

Fast solvers for Connection Laplacians

[Kyng-Lee-Peng-S-Spielman ’16]

For any connection Laplacian M, subset A that is strongly diagonally dominant, in time $\widetilde{O_\varepsilon}(m)$, can compute a connection laplacian $\widetilde{M}$ on V\A s.t. $\widetilde{M}$ has $\widetilde{O_\varepsilon}(m)$ edges, and

$$\widetilde{M} \approx_\varepsilon Sc(M, V\backslash \mathrm{A})$$

Fast solvers for Connection Laplacians

Combined with sparsification, this gives the only known nearly-linear time solver for Connection Laplacians

[Kyng-Lee-Peng-S-Spielman ’16]
For any connection Laplacian M, with m edges
can solve $Mx = b$ ε–approximately in $\tilde{O}(m \log {}^{1}/_{\varepsilon})$

Where do we go from here?

Approximate Schur complements for other problems? Max-flow?

Faster solvers for more general families of systems? Truss matrices?

[Kyng-Zhang ‘17] Fast solvers for matrices with structure similar to connection Laplacians, imply fast solvers for all matrices

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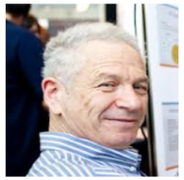

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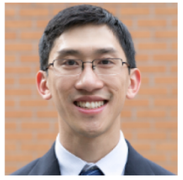

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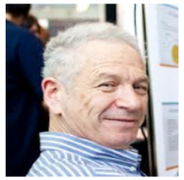

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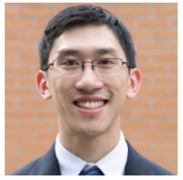

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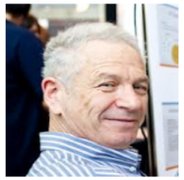

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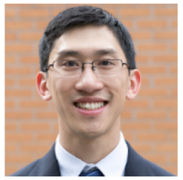

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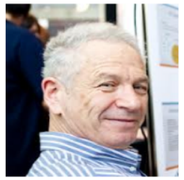

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Graph Theory,
Combinatorics

Aleksandar Nikolov
Algorithms,
Discrepancy Theory,
Privacy

Toniann Pitassi
Complexity Theory,
Proof Complexity

Charles Rackoff
Cryptography,
Complexity Theory

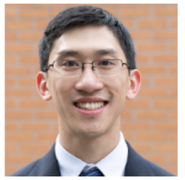
Benjamin Rossman
Circuit Complexity,
Logic

Sushant Sachdeva
Algorithms,
Optimization,
Learning

Nisarg Shah
Mechanism Design,
Game Theory

Sam Toueg
Distributed Computing

Alasdair Urquhart
Complexity of Proofs,
Logic,
History of Logic



Henry Yuen
Quantum Computing,
Quantum Cryptography,
Complexity Theory

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