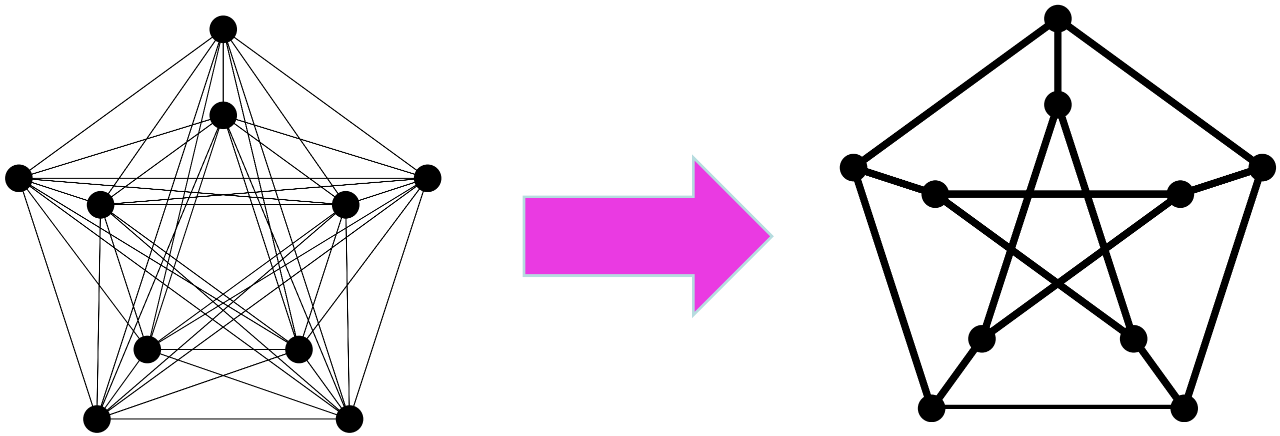
Laplacian Matrices of Graphs: Algorithms and Applications



Daniel A. Spielman

Yale Institute For Network Science

ICML, June 21, 2016

Outline

- Laplacians
  - Interpolation on graphs
  - Spring networks
  - Clustering
  - Isotonic regression
- Sparsification
- Solving Laplacian Equations
  - Best results
  - The simplest algorithm

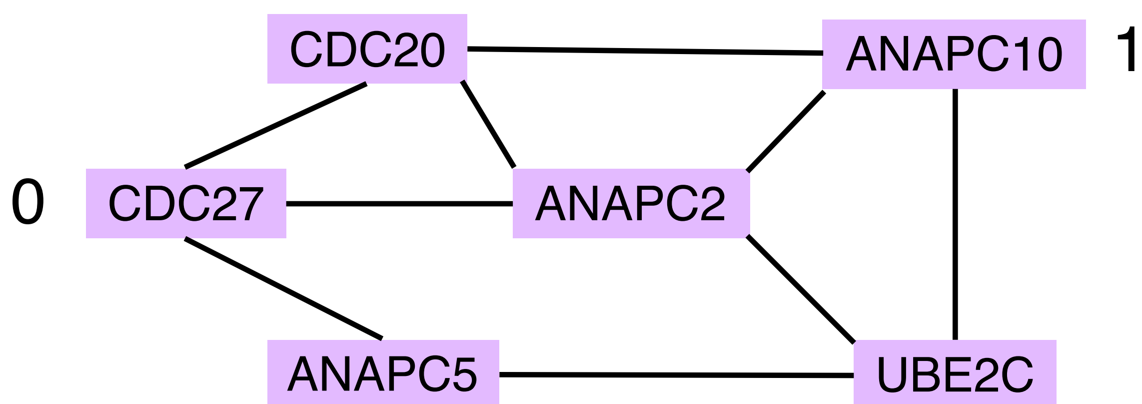
Interpolation on Graphs

(Zhu,Ghahramani,Lafferty '03)

Interpolate values of a function at all vertices from given values at a few vertices.

Minimize $$\sum_{(i,j) \in E} (x(i) - x(j))^2$$

Subject to given values



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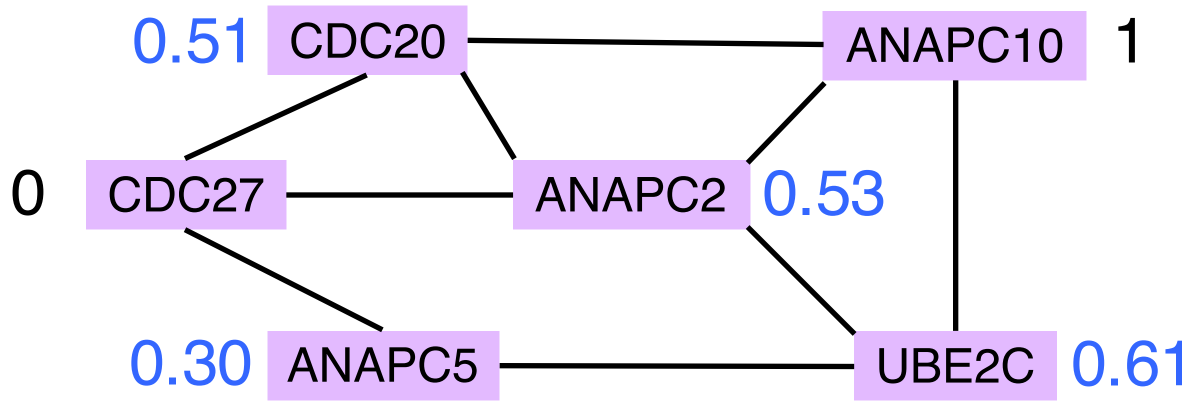

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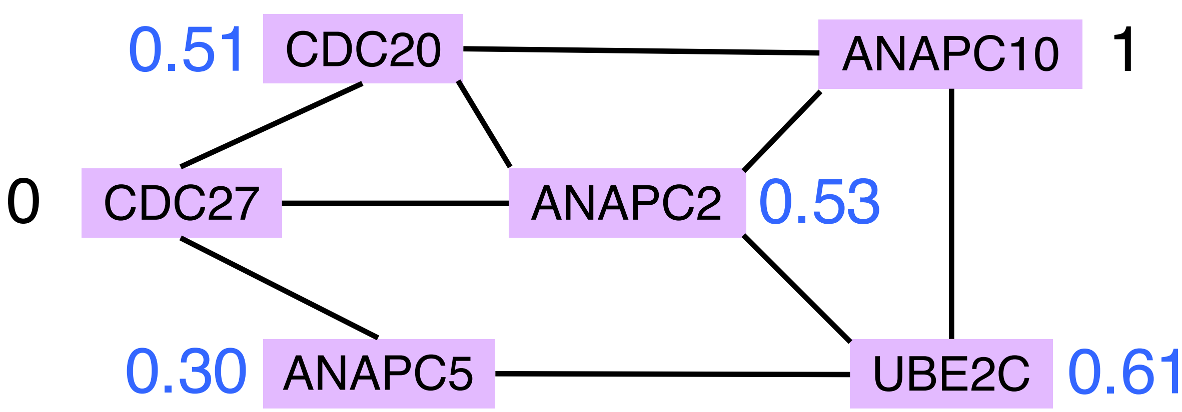
(Zhu,Ghahramani,Lafferty '03)

Interpolate values of a function at all vertices from given values at a few vertices.

Minimize $$\sum_{(i,j)\in E} (x(i) - x(j))^2 = x^T L_G x$$

Subject to given values



Take derivatives. Minimize by solving Laplacian

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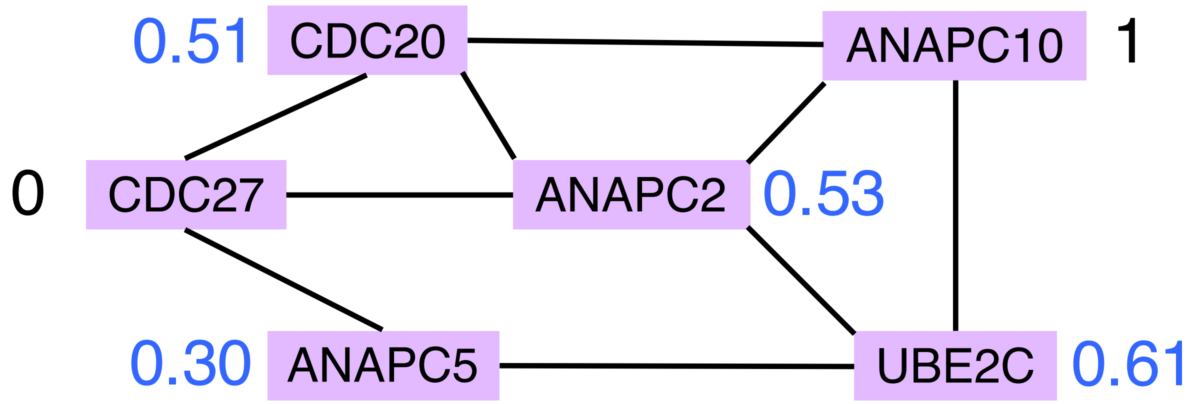


The Laplacian Quadratic Form

$$\sum_{(i,j)\in E} (x(i) - x(j))^2$$

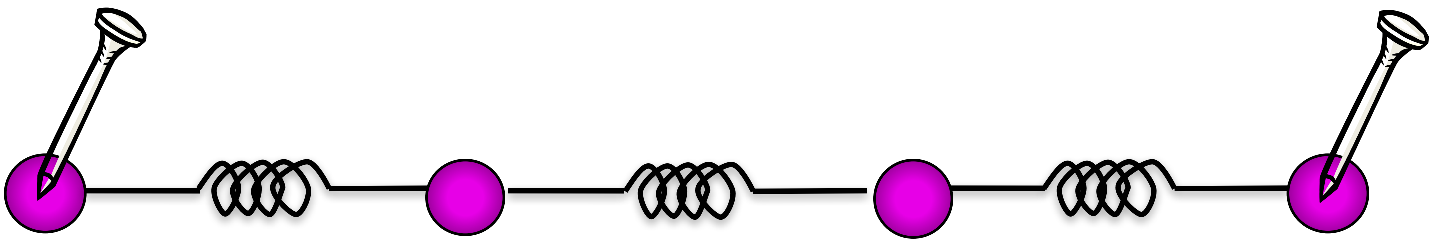
The Laplacian Matrix of a Graph

$$x^T L_G x = \sum_{(i,j) \in E} (x(i) - x(j))^2$$

Spring Networks

View edges as rubber bands or ideal linear springs

Nail down some vertices, let rest settle



In equilibrium, nodes are averages of neighbors.

Spring Networks

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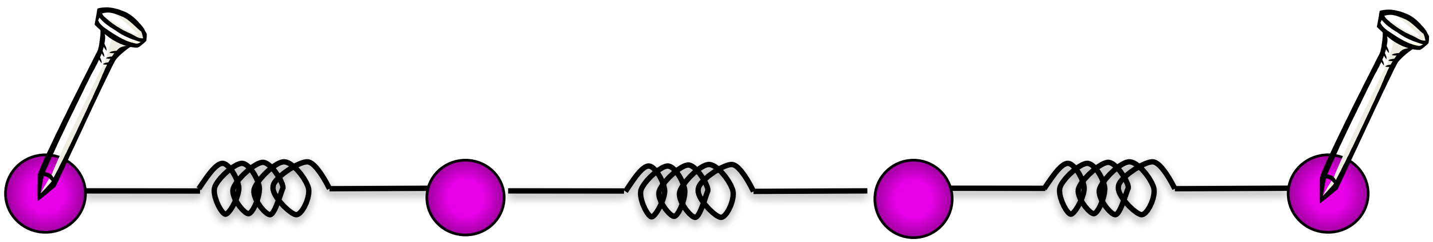
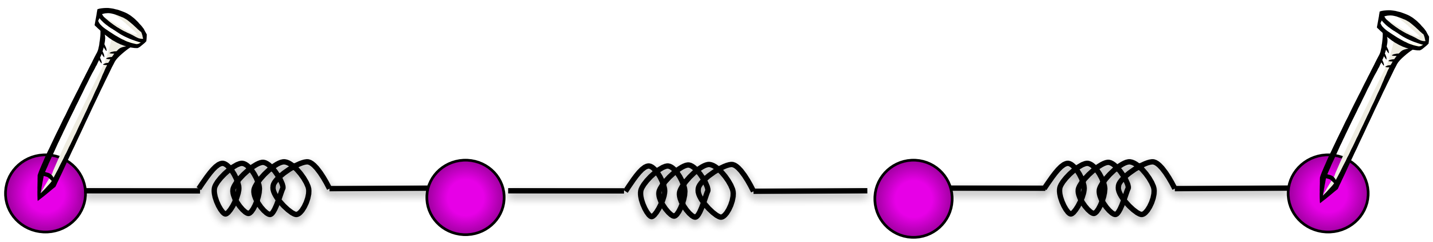


When stretched to length ℓ

potential energy is $\ell^2/2$

Spring Networks

Nail down some vertices, let rest settle



Physics: position minimizes total potential energy

$$\frac{1}{2} \sum_{(i,j) \in E} (x(i) - x(j))^2$$

subject to boundary constraints (nails)

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Interpolate values of a function at all vertices from given values at a few vertices.

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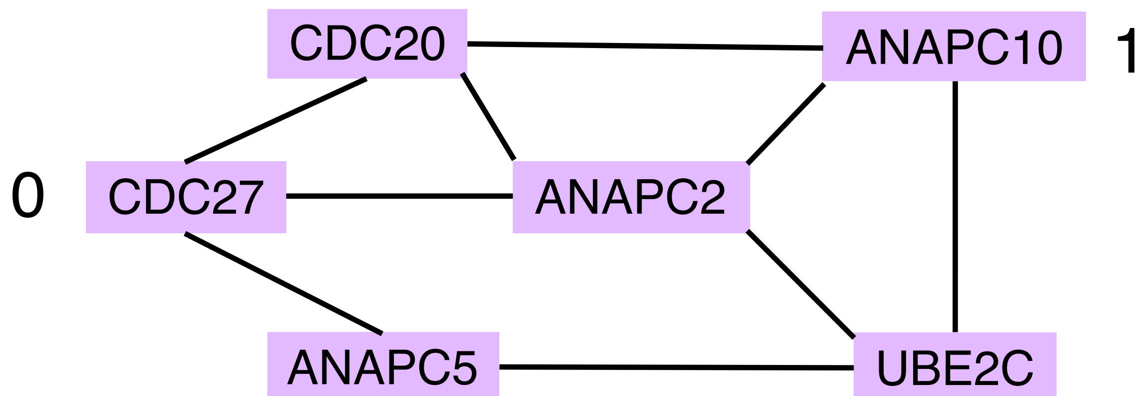

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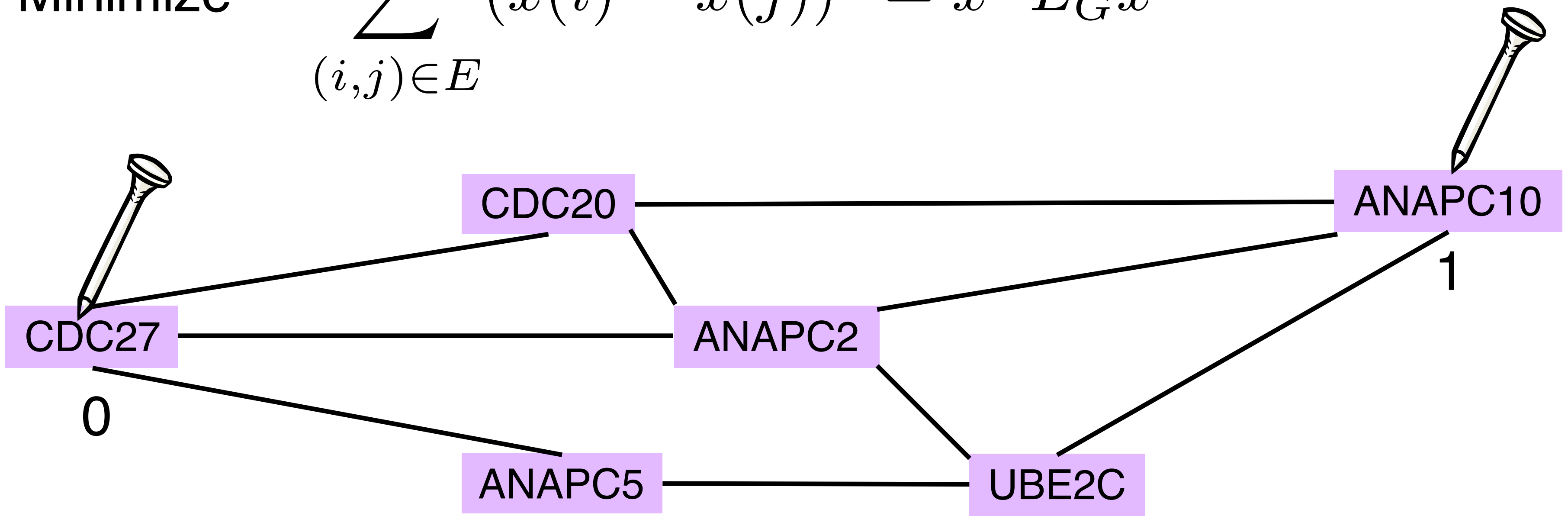

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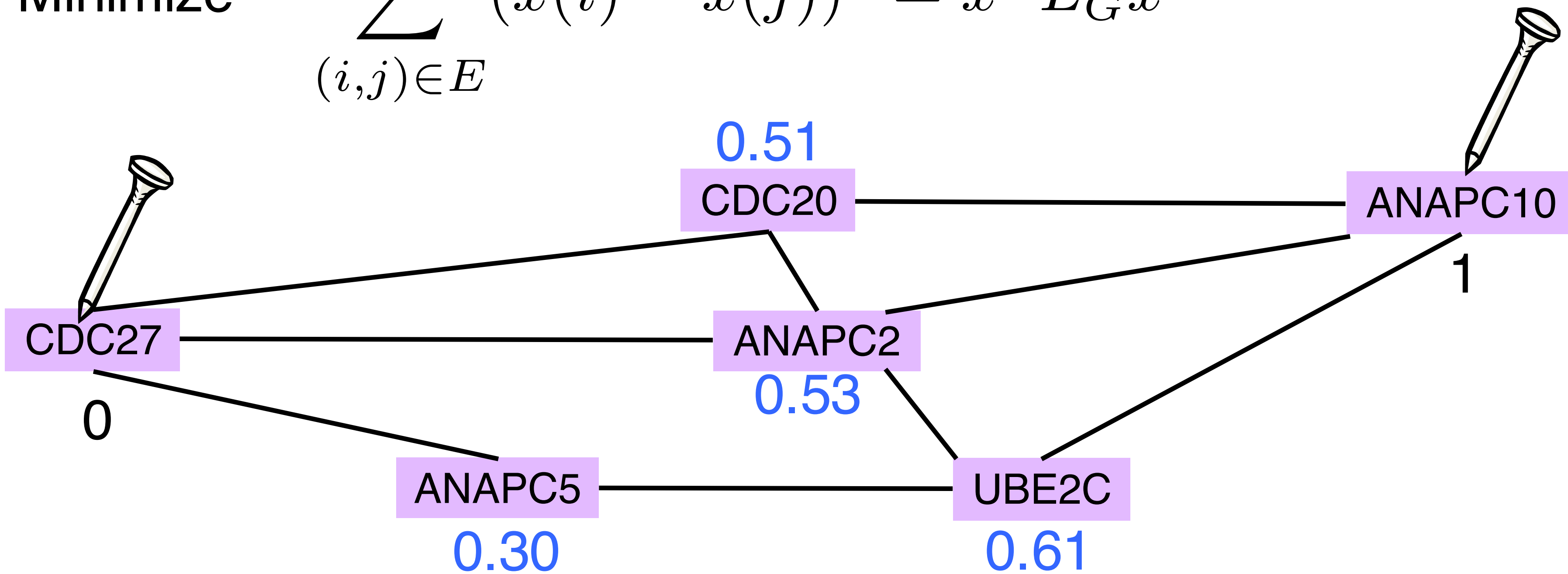
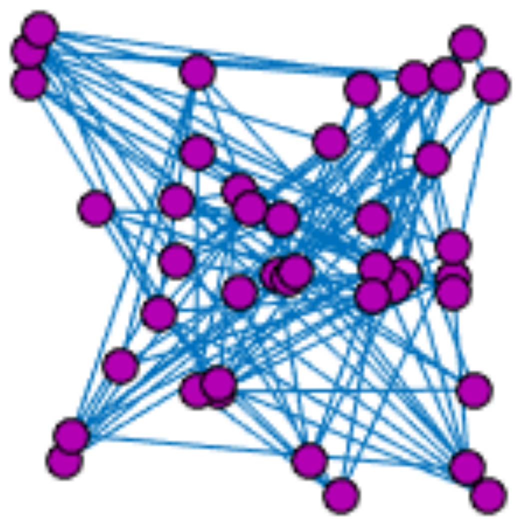


In the solution, variables are the average of their neighbors

Drawing by Spring Networks (Tutte '63)



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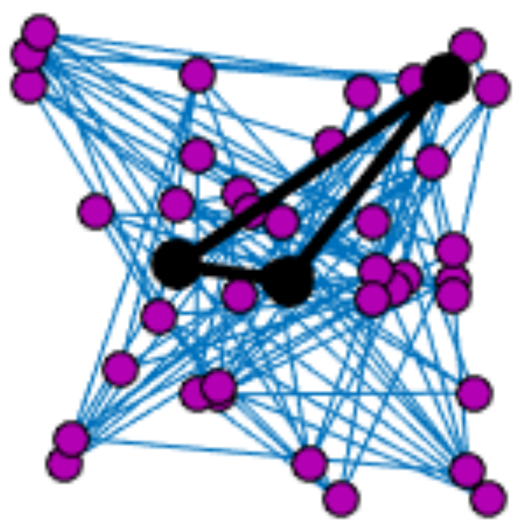

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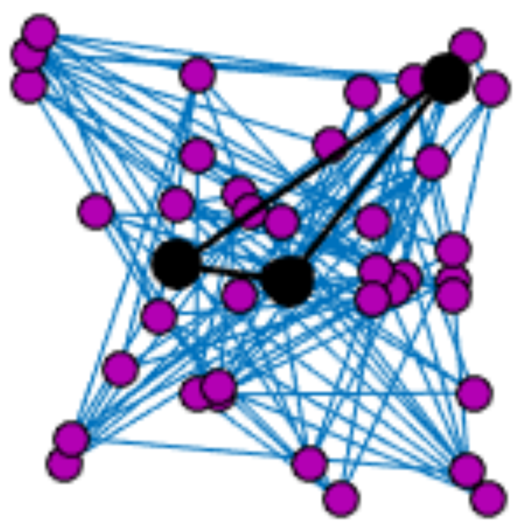

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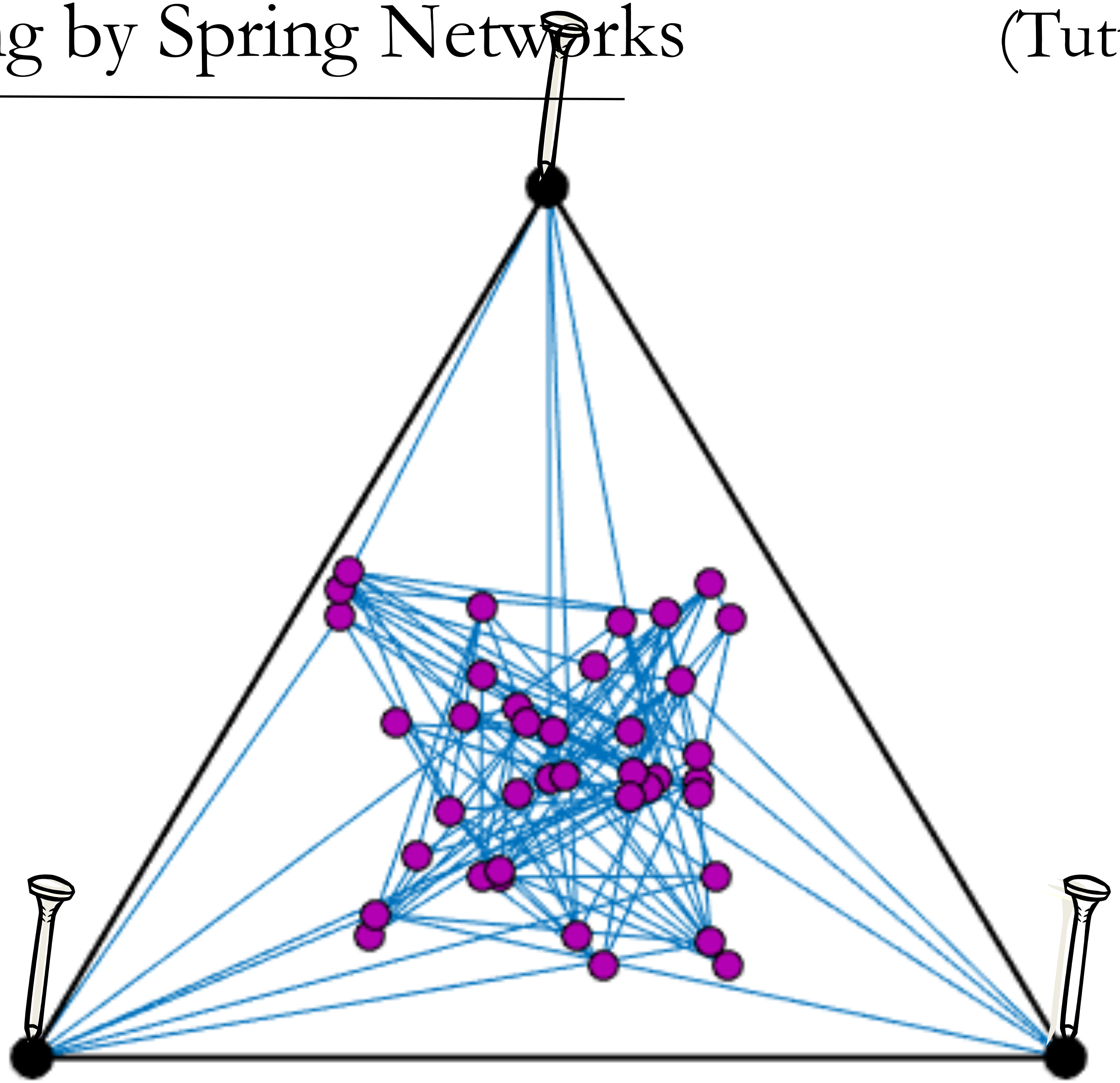

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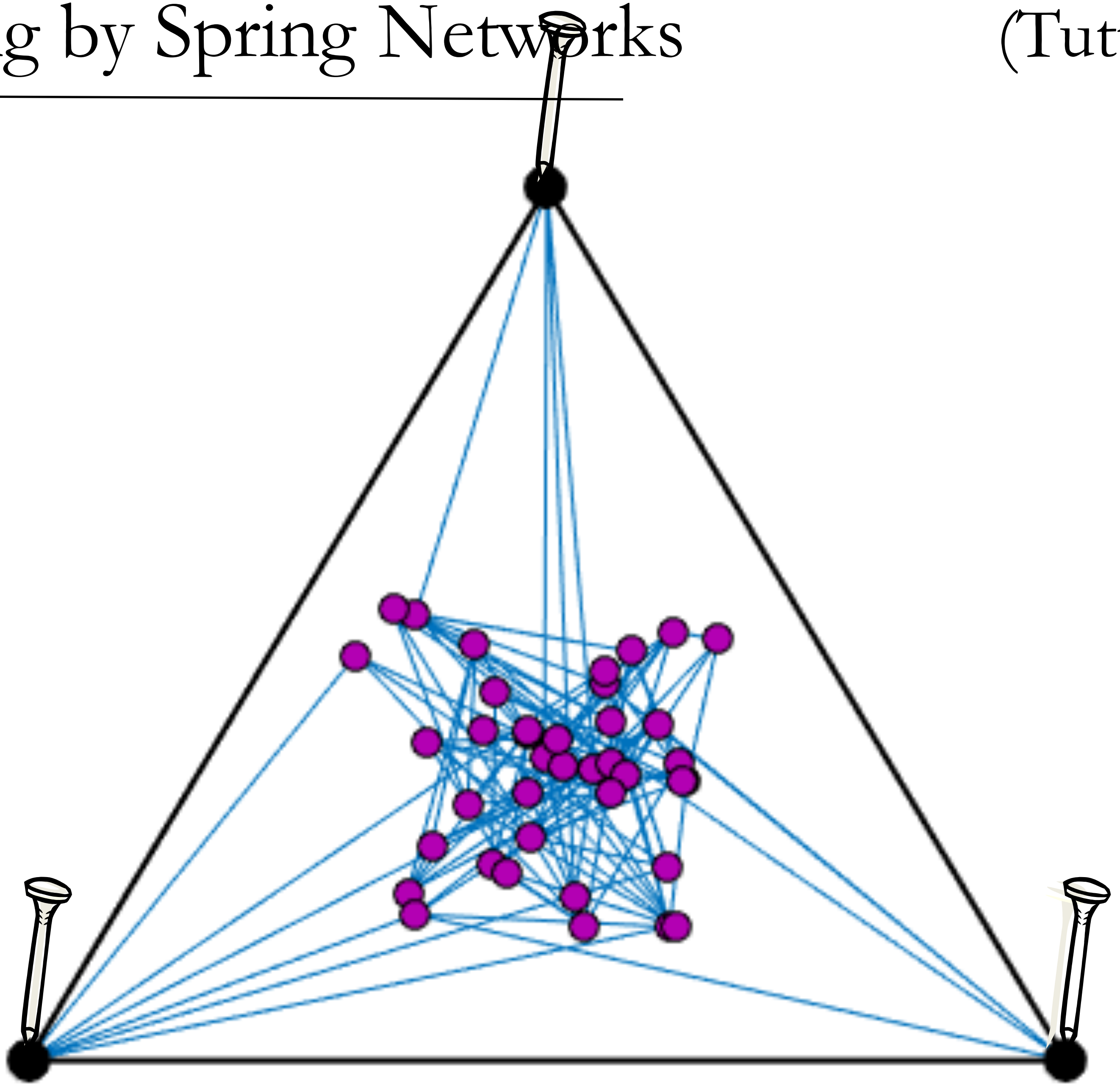
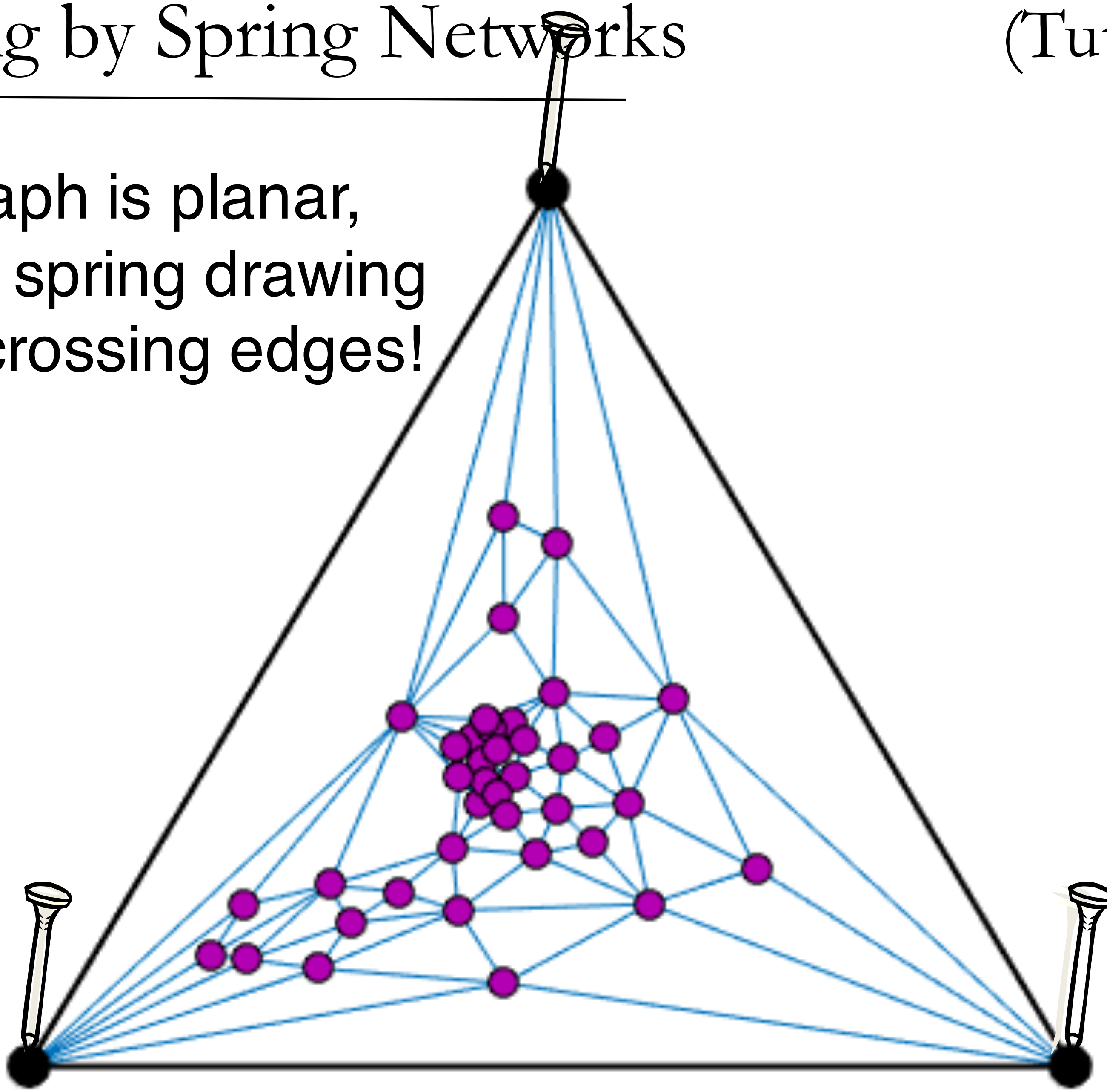


Drawing by Spring Networks (Tutte '63)

If the graph is planar, then the spring drawing has no crossing edges!



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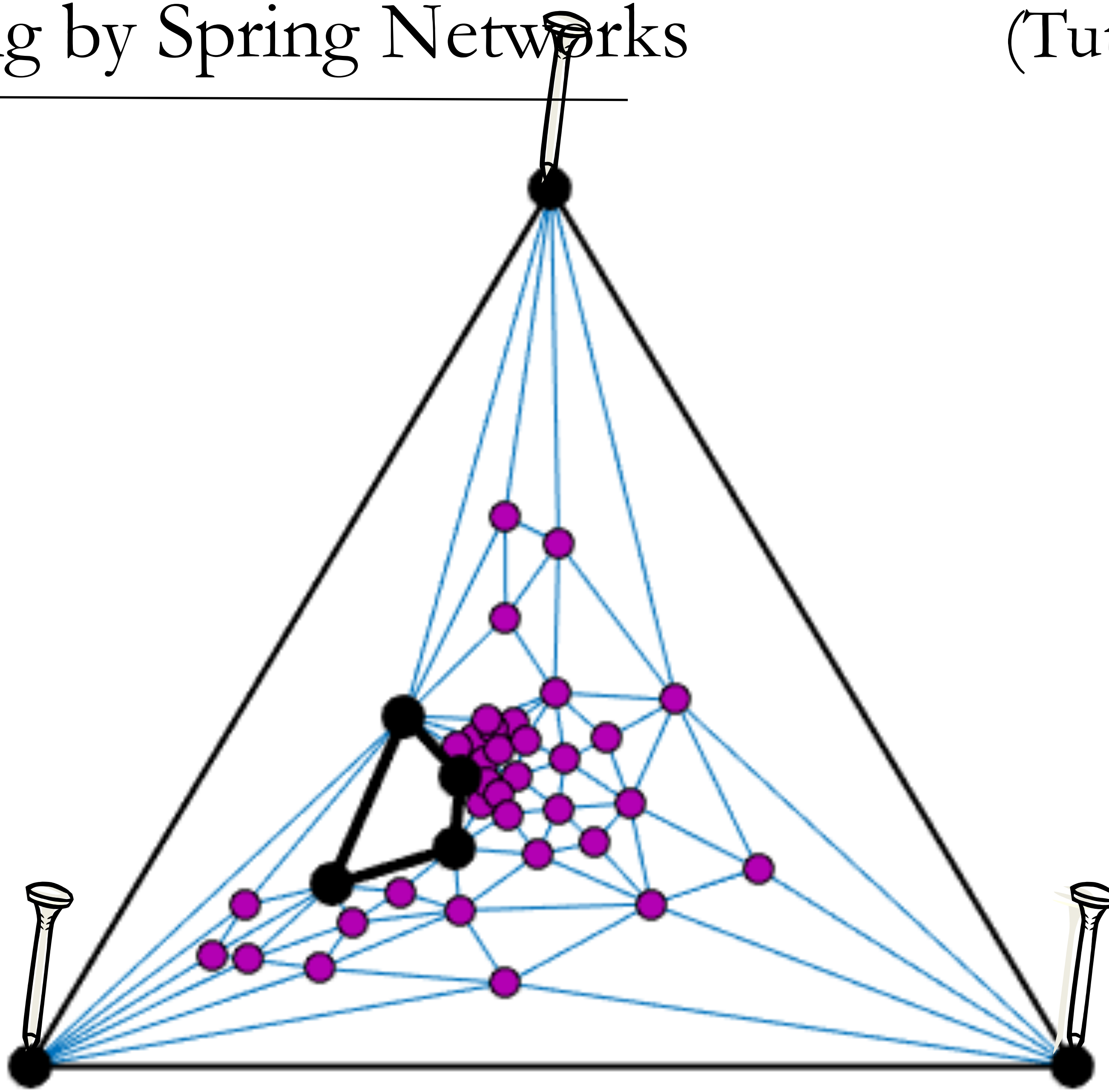

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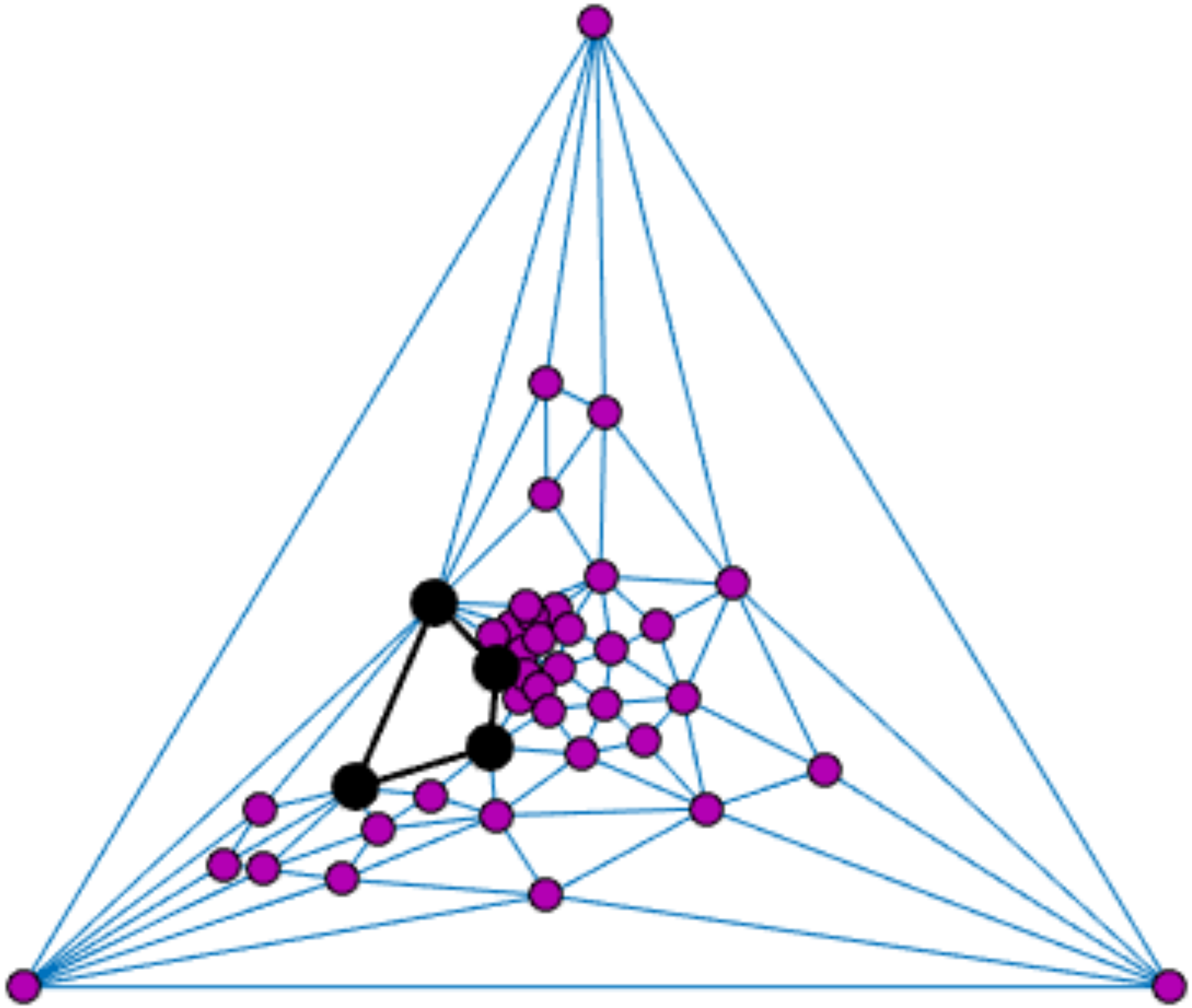

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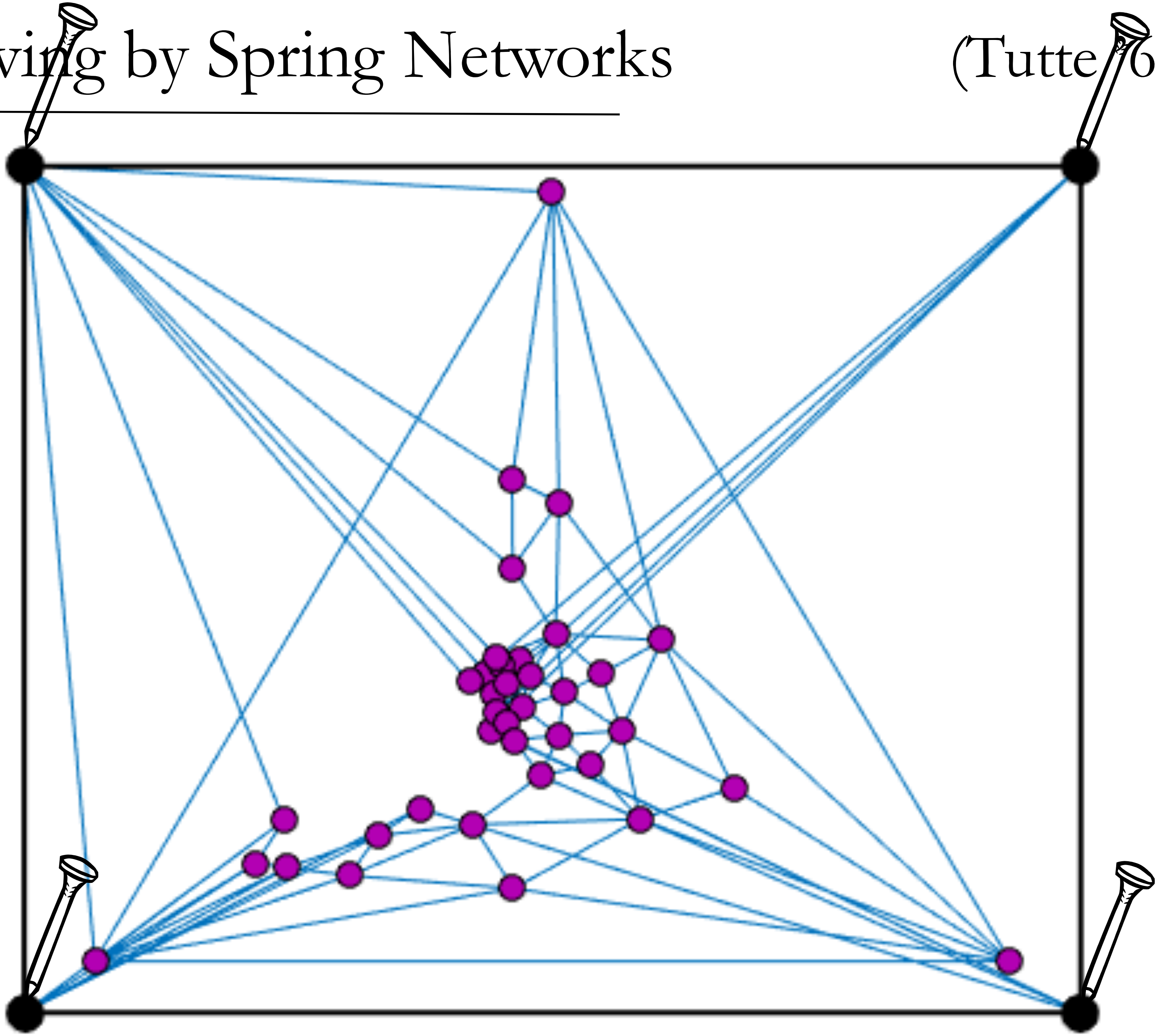

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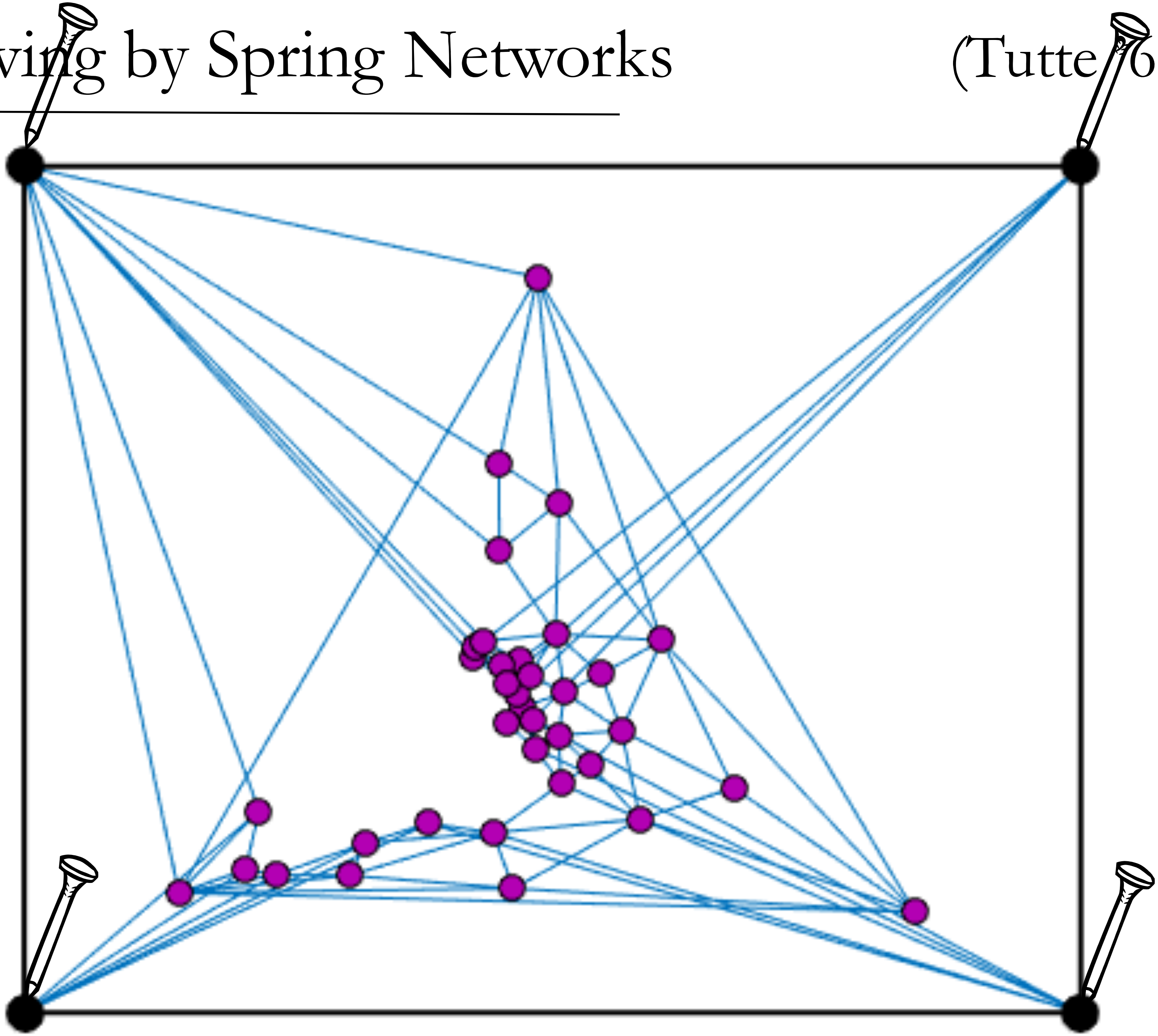

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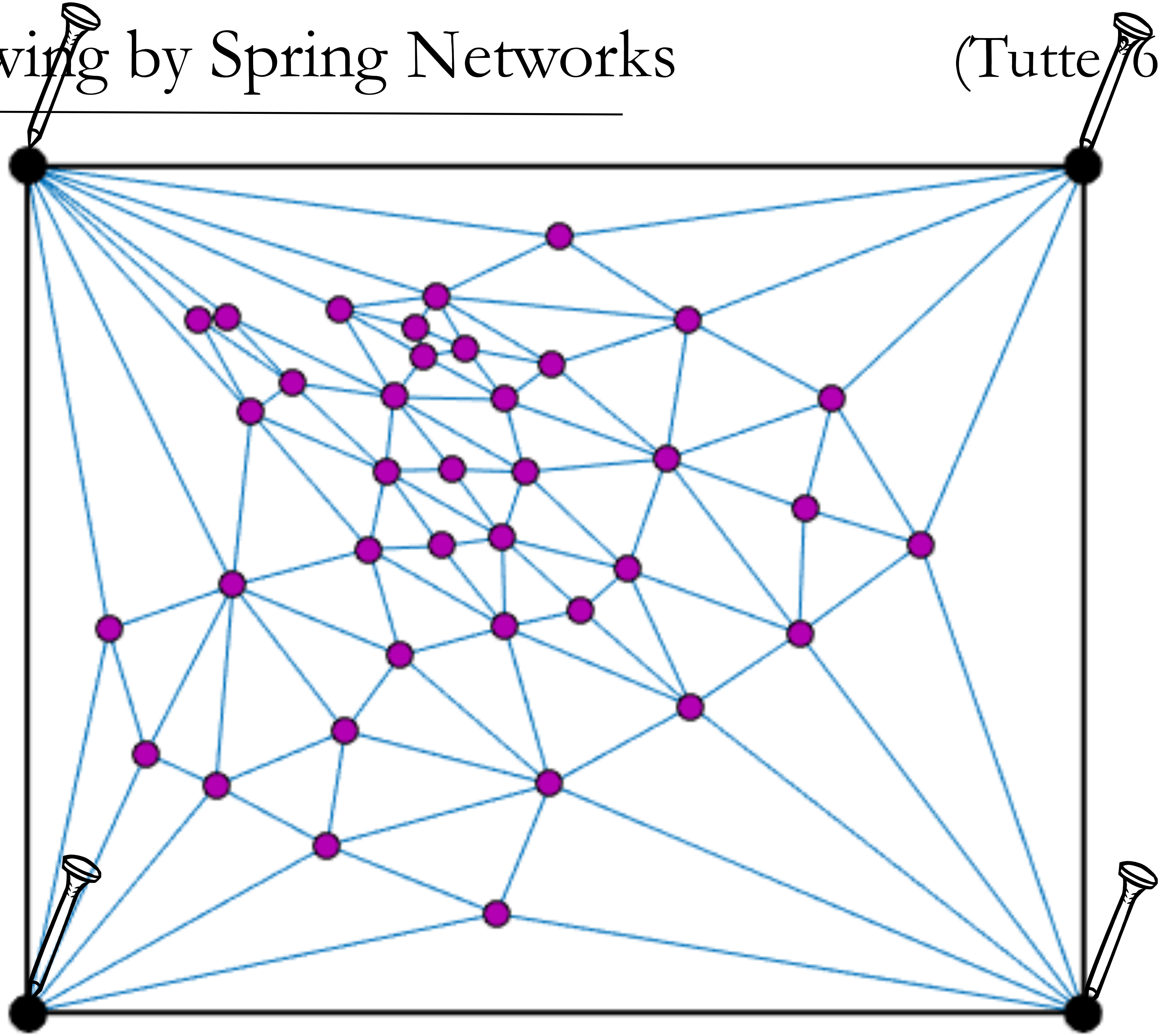
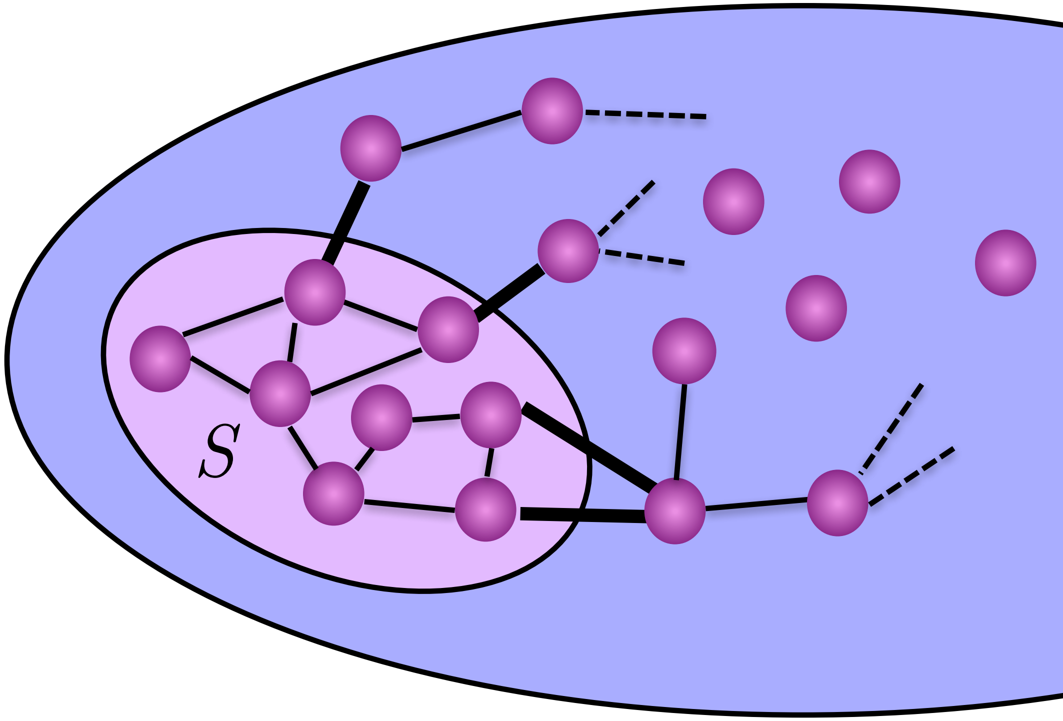


Measuring boundaries of sets

Boundary: edges leaving a set

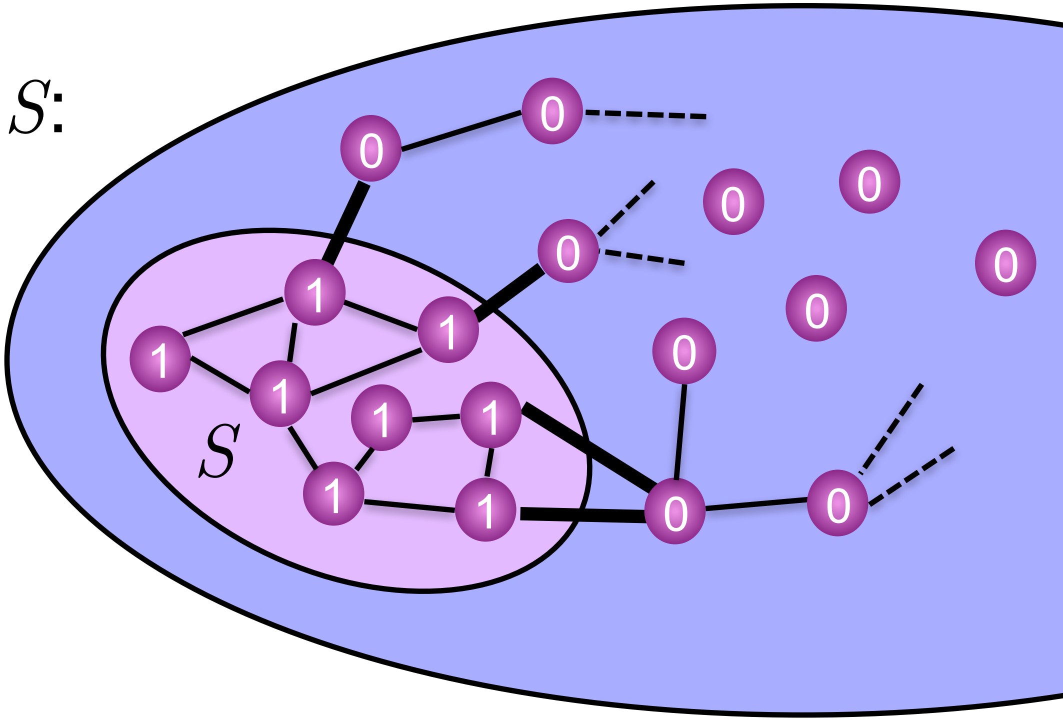


Measuring boundaries of sets

Boundary: edges leaving a set

Characteristic Vector of S:

$$x(i) = \begin{cases} 1 & i \text{ in } S \\ 0 & i \text{ not in } S \end{cases}$$



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Characteristic Vector of S:

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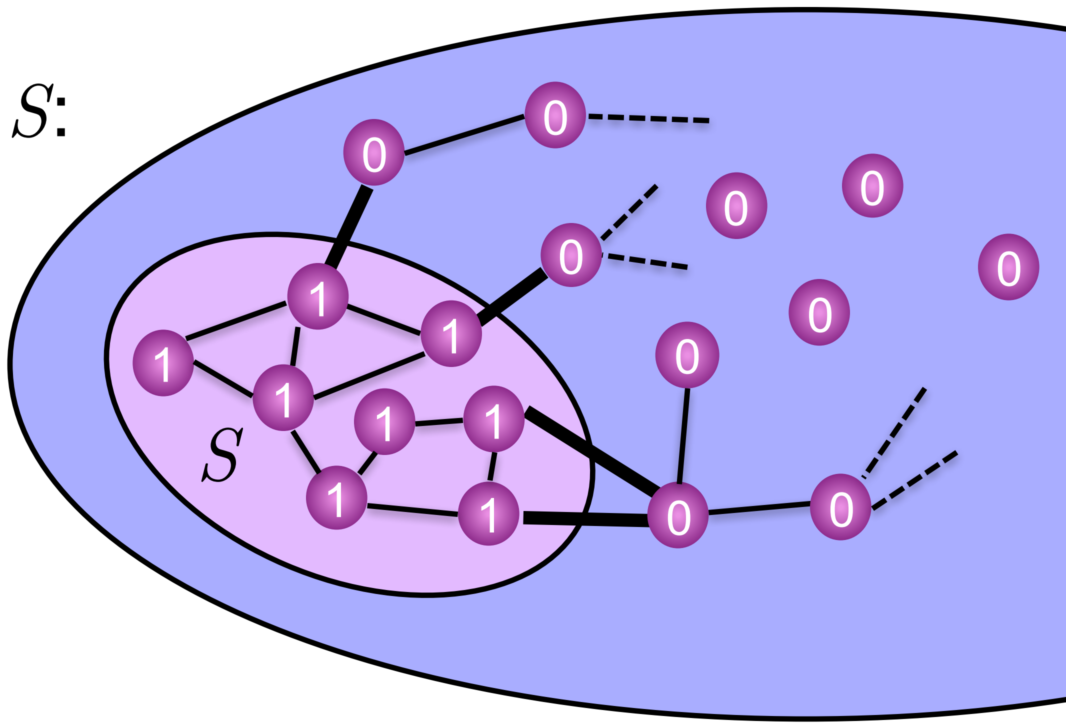
$$\sum_{(i,j) \in E} (x(i) - x(j))^2$$

$$= |\text{boundary}(S)|$$



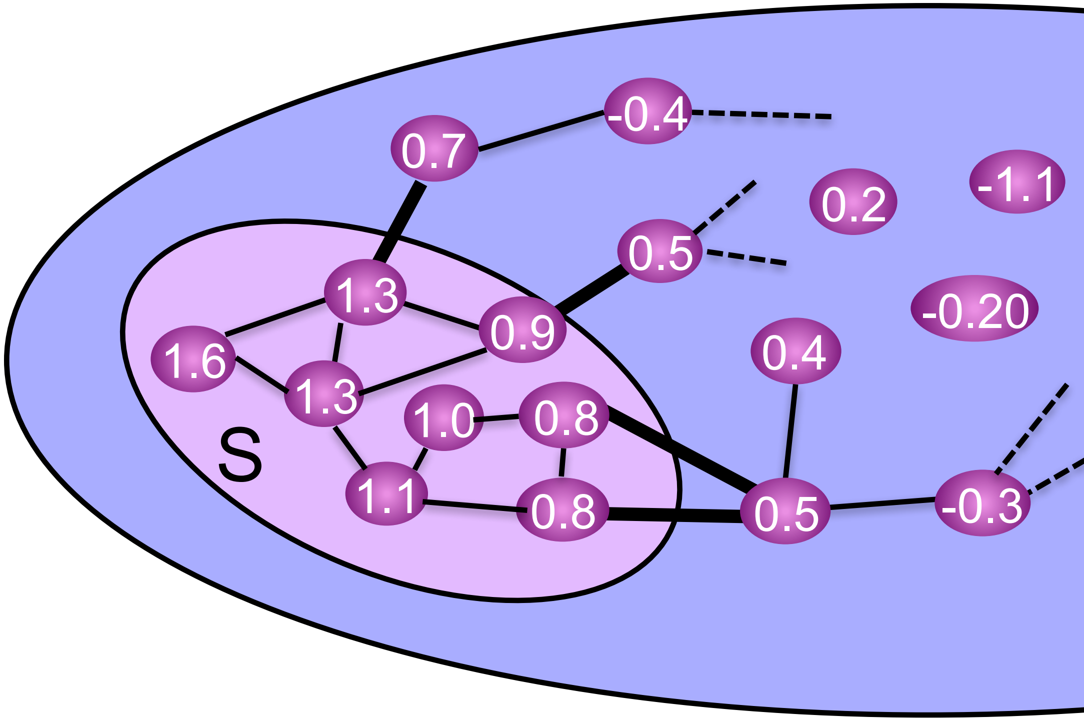
Spectral Clustering and Partitioning

Find large sets of small boundary

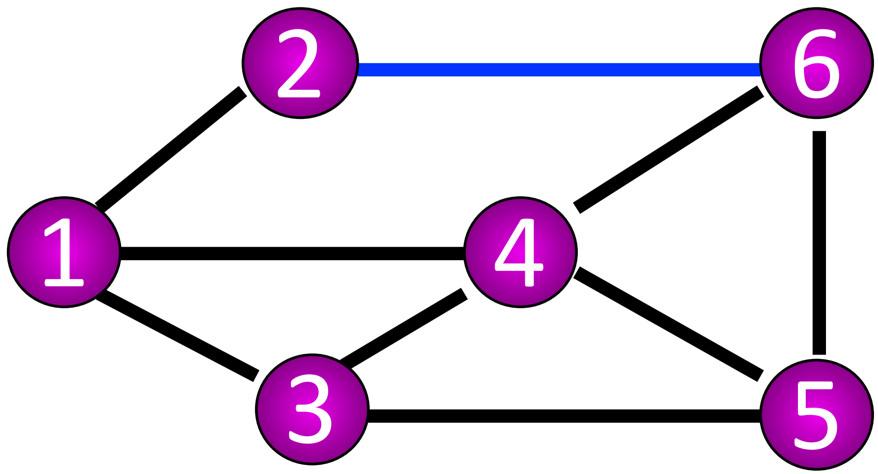
Heuristic to find
x with $x^T L_G x$ small

Compute eigenvector
$$L_G v_2 = \lambda_2 v_2$$

Consider the level sets



The Laplacian Matrix of a Graph



$$\begin{pmatrix} 3 & -1 & -1 & -1 & 0 & 0 \\ -1 & 2 & 0 & 0 & 0 & -1 \\ -1 & 0 & 3 & -1 & -1 & 0 \\ -1 & 0 & -1 & 4 & -1 & -1 \\ 0 & 0 & -1 & -1 & 3 & -1 \\ 0 & -1 & 0 & -1 & -1 & 3 \end{pmatrix}$$

Symmetric

Non-positive off-diagonals

Diagonally dominant

The Laplacian Matrix of a Graph

$$x^T L_G x = \sum_{(i,j) \in E} (x(i) - x(j))^2$$

$$x(i) - x(j) = \begin{pmatrix} 1 & -1 \end{pmatrix} \begin{pmatrix} x(i) \\ x(j) \end{pmatrix}$$

$$(x(i) - x(j))^2 = \begin{pmatrix} x(i) \\ x(j) \end{pmatrix}^T \begin{pmatrix} 1 \\ -1 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix}^T \begin{pmatrix} x(i) \\ x(j) \end{pmatrix}$$

$$= \begin{pmatrix} x(i) \\ x(j) \end{pmatrix}^T \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \begin{pmatrix} x(i) \\ x(j) \end{pmatrix}$$

Laplacian Matrices of Weighted Graphs

$$x^T L_G x = \sum_{(i,j)\in E} w_{i,j}(x(i) - x(j))^2$$

$$L_G = \sum_{(i,j)\in E} w_{i,j}(b_{i,j} b_{i,j}^T)$$ where $b_{i,j} = e_i - e_j$

Laplacian Matrices of Weighted Graphs

$$L_G = \sum_{(i,j) \in E} w_{i,j} (b_{i,j} b_{i,j}^T) \qquad \text{where } b_{i,j} = e_i - e_j$$

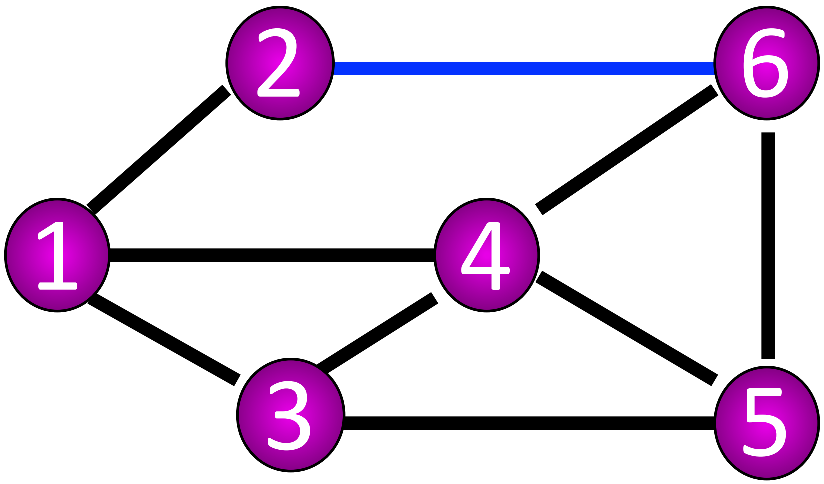
$$L_G = B^T W B$$

B is the signed edge-vertex adjacency matrix with one row for each $b_{i,j}$

W is the diagonal matrix of weights $w_{i,j}$

Laplacian Matrices of Weighted Graphs

$$L_G = \sum_{(i,j)\in E} w_{i,j}(b_{i,j}b_{i,j}^T) \qquad L_G = B^T W B$$



$$B = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & -1 \\ 1 & 0 & 0 & -1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & -1 \\ 1 & 0 & -1 & 0 & 0 & 0 \\ 0 & 0 & 1 & -1 & 0 & 0 \\ 0 & 0 & 1 & 0 & -1 & 0 \\ 0 & 0 & 0 & 1 & -1 & 0 \\ 0 & 0 & 0 & 0 & 1 & -1 \end{pmatrix}$$

Quickly Solving Laplacian Equations

S,Teng '04: Using low-stretch trees and sparsifiers

$$O(m \log^c n \log \epsilon^{-1})$$

Where m is number of non-zeros and n is dimension

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Cohen, Kyng, Pachocki, Peng, Rao '14:

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Good code:

LAMG (lean algebraic multigrid) – Livne-Brandt

CMG (combinatorial multigrid) – Koutis

Quickly Solving Laplacian Equations

S,Teng '04: Using low-stretch trees and sparsifiers

$$O(m \log^c n \log \epsilon^{-1})$$

An ϵ-accurate solution to $L_G x = b$
is an x satisfying

$$\|x - x^*\|_{L_G} \leq \epsilon \|x^*\|_{L_G}$$

where $\|v\|_{L_G} = \sqrt{v^T L_G v} = ||L_G^{1/2} v||$

Quickly Solving Laplacian Equations

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$$\|x - x^*\|_{L_G} \leq \epsilon \|x^*\|_{L_G}$$

Allows fast computation of eigenvectors
corresponding to small eigenvalues.

Laplacians in Linear Programming

Laplacians appear when solving Linear Programs on
on graphs by Interior Point Methods

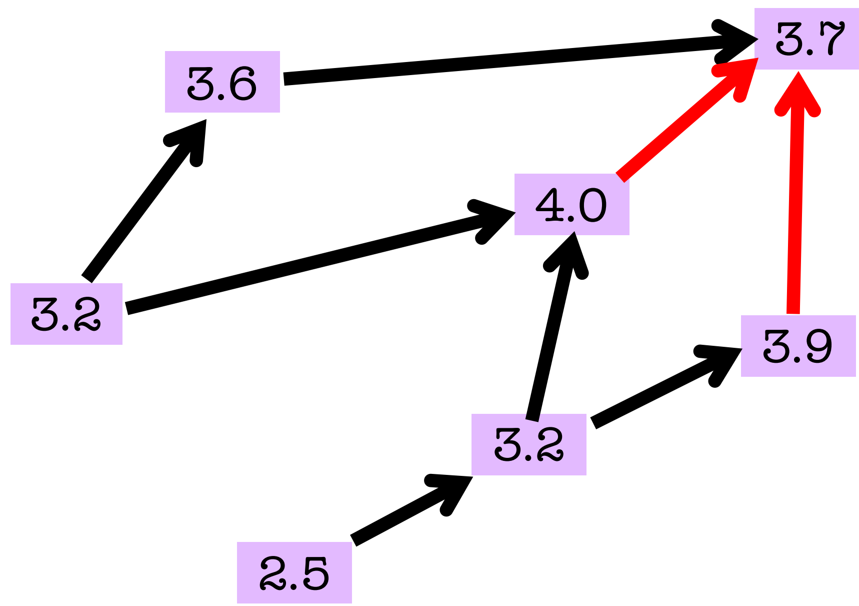
Lipschitz Learning : regularized interpolation on graphs
(Kyng, Rao, Sachdeva,S '15)

Maximum and Min-Cost Flow (Daitch, S '08, Mądry '13)

Shortest Paths (Cohen, Mądry, Sankowski, Vladu '16)

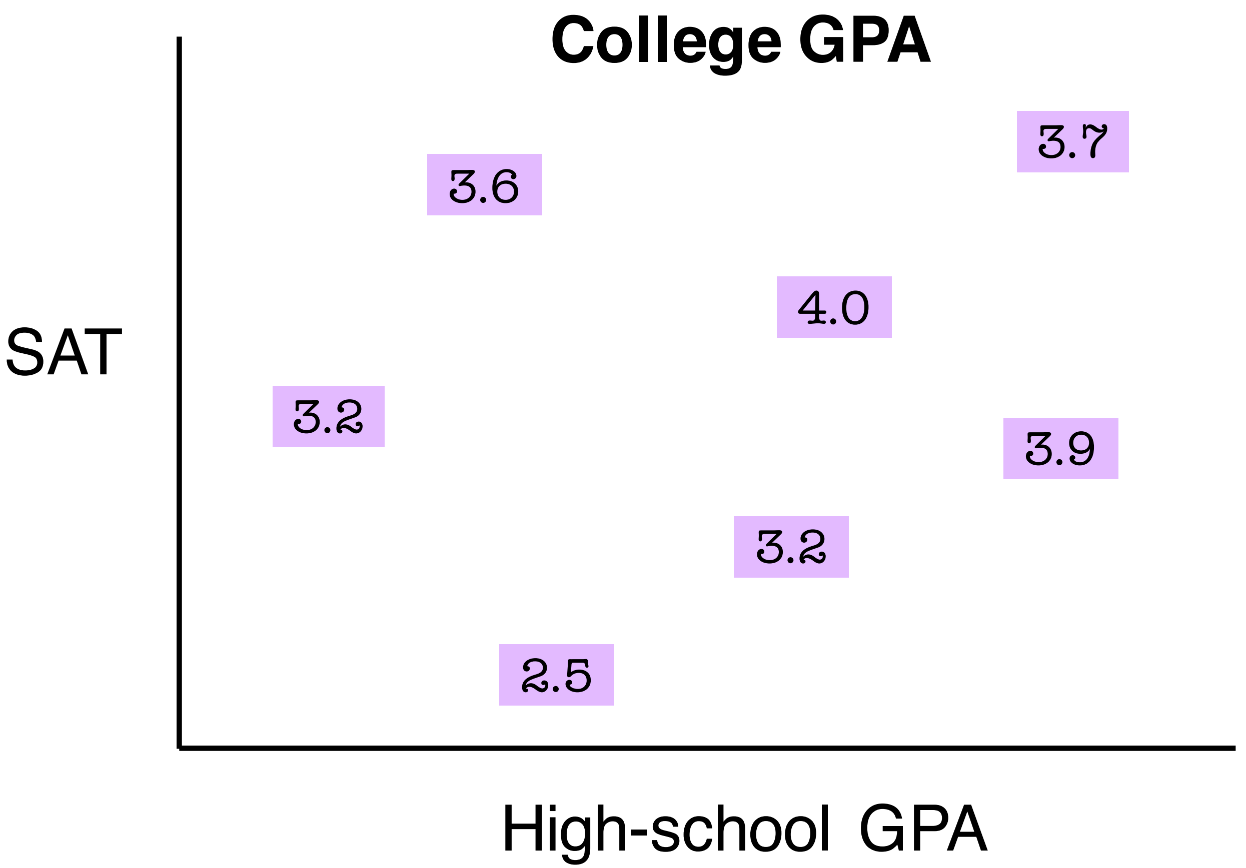
Isotonic Regression (Kyng, Rao, Sachdeva '15)

Isotonic Regression (Ayer et. al. '55)



A function $x : V \to \mathbb{R}$ is isotonic with respect to a directed acyclic graph if x increases on edges.

Isotonic Regression (Ayer et. al. '55)



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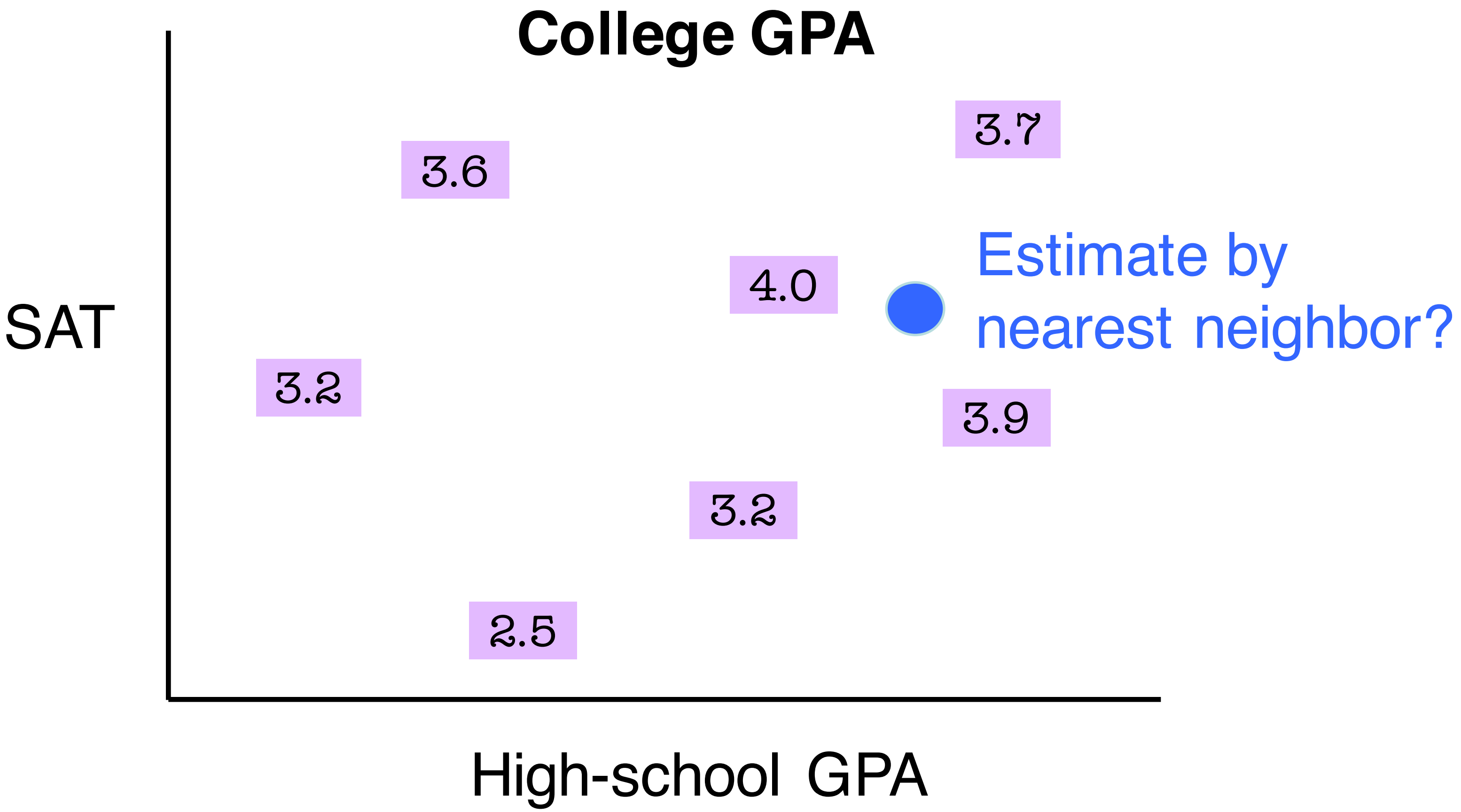

Isotonic Regression

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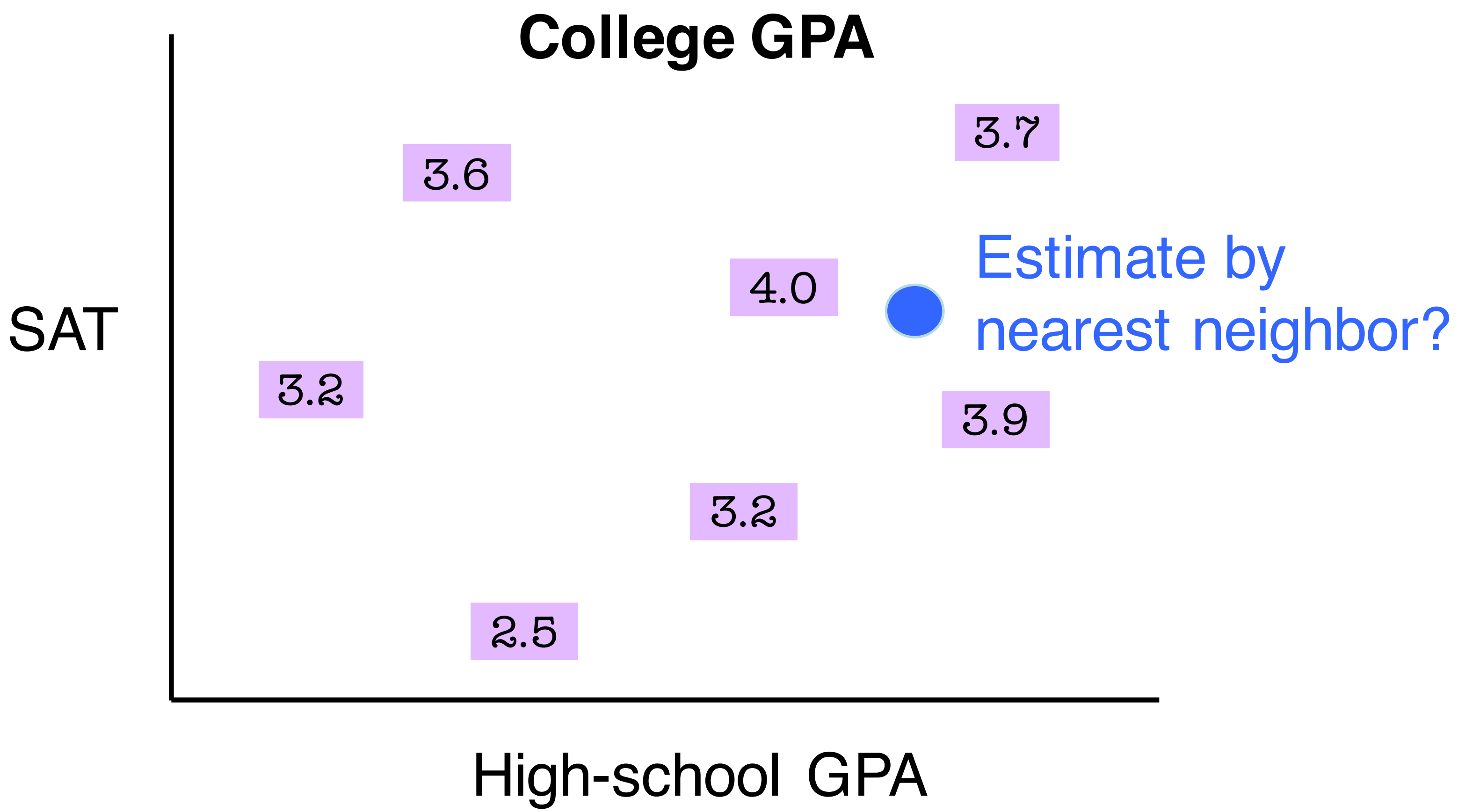
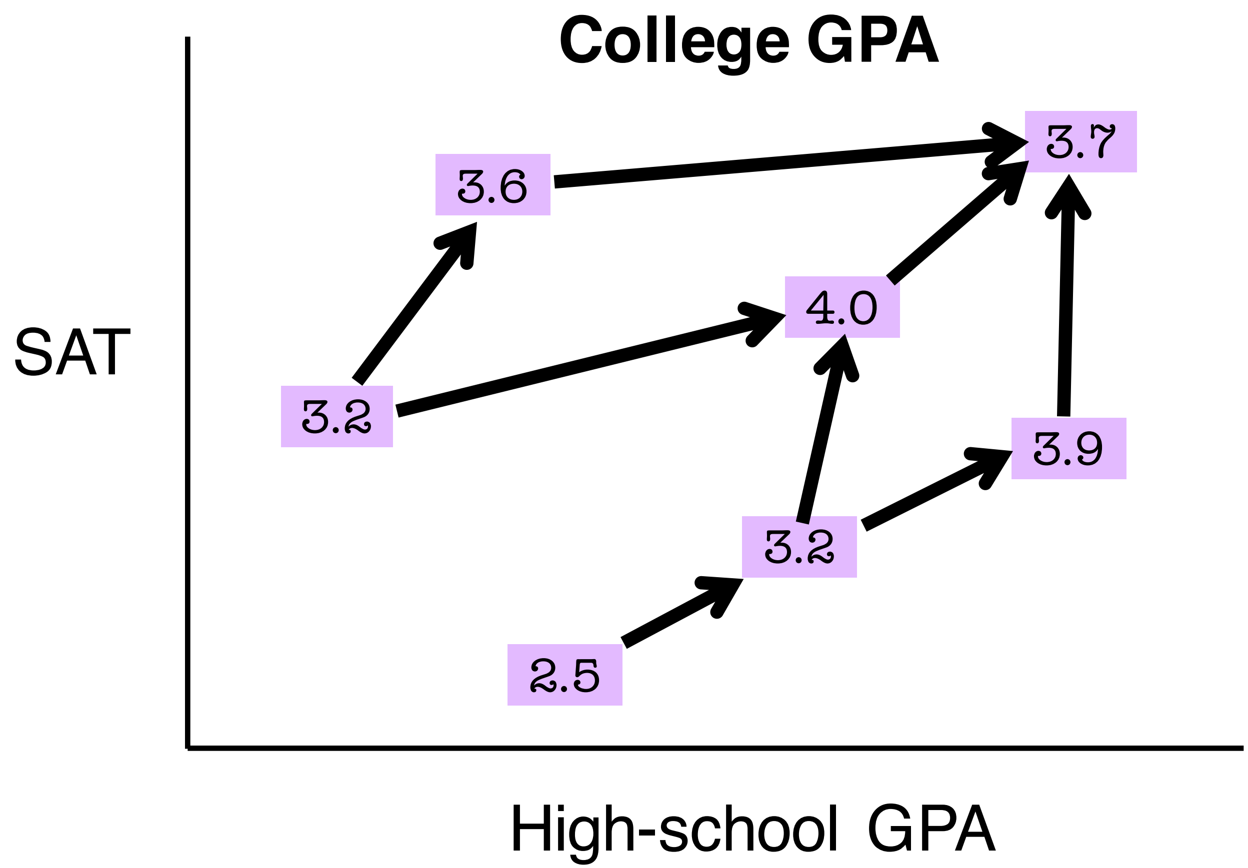


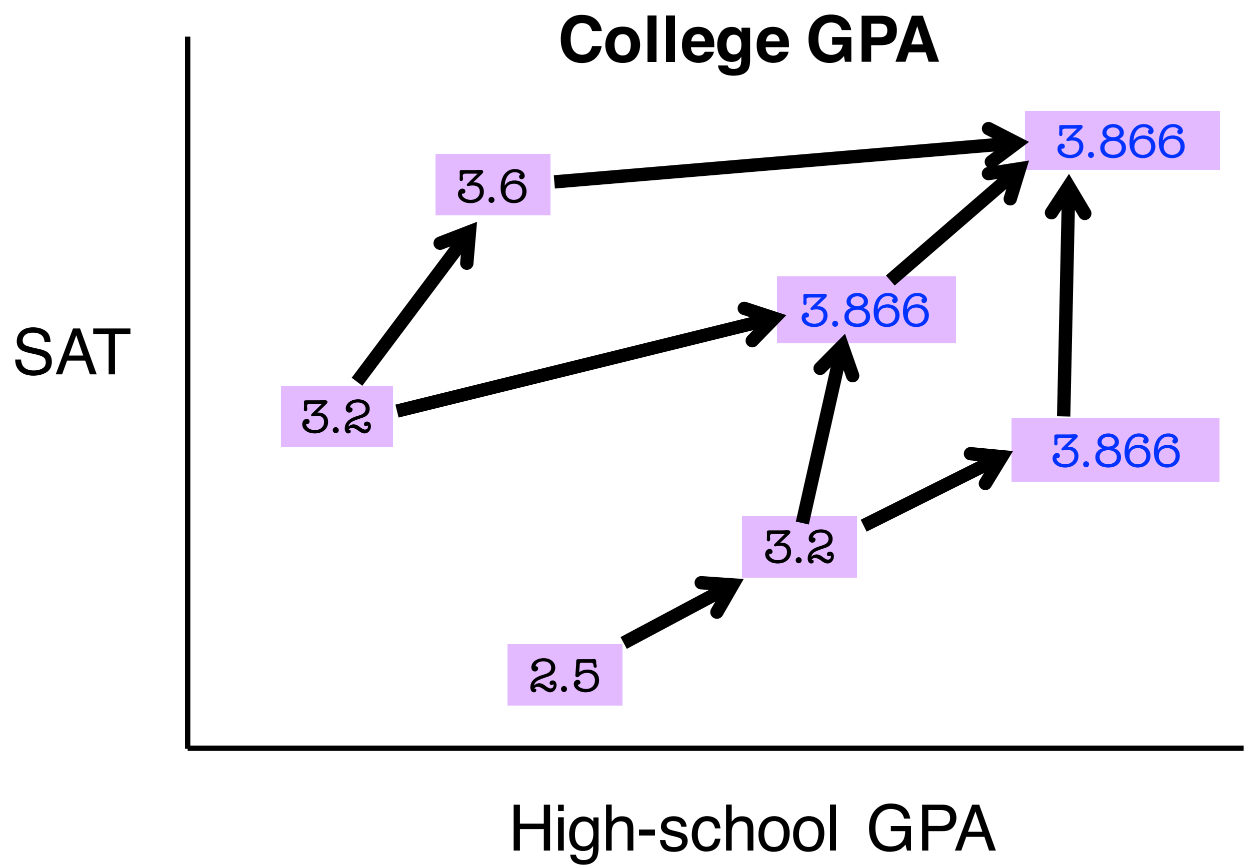
We want the estimate to be monotonically increasing

Isotonic Regression (Ayer et. al. '55)



Given $y : V \to \mathbb{R}$ find the isotonic x minimizing $\|x - y\|$

Isotonic Regression (Ayer et. al. '55)



Given $y : V \to \mathbb{R}$ find the isotonic x minimizing $\|x - y\|$

Fast IPM for Isotonic Regression

(Kyng, Rao, Sachdeva '15)

Given $y : V \to \mathbb{R}$ find the isotonic x minimizing $\|x - y\|_1$

Fast IPM for Isotonic Regression

(Kyng, Rao, Sachdeva '15)

Given $y : V \to \mathbb{R}$ find the isotonic x minimizing $\|x - y\|_1$

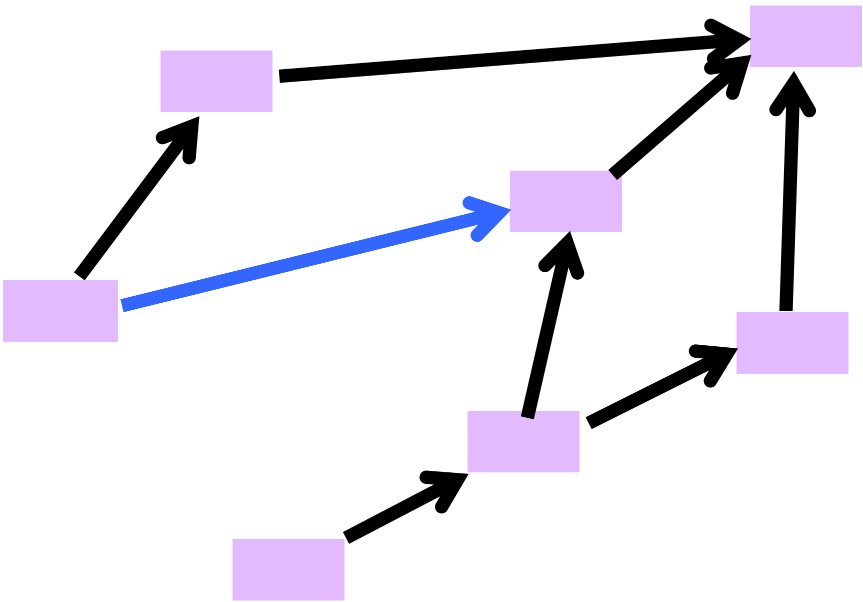
or $\|x - y\|_p$ for any $p > 1$

in time $O(m^{3/2} \log^3 m)$

Linear Program for Isotonic Regression

Signed edge-vertex incidence matrix

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



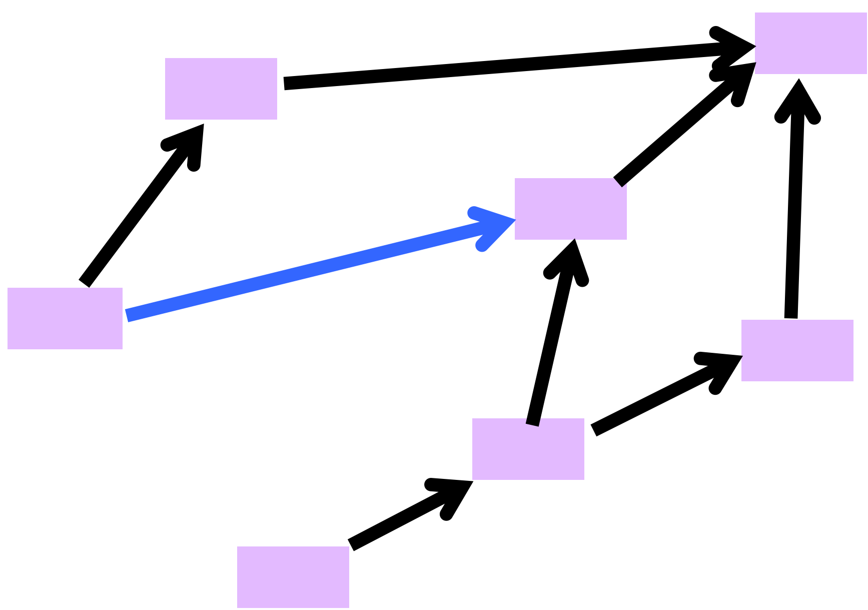
x is isotonic if $Bx \leq 0$

Linear Program for Isotonic Regression

Given y, minimize $\|x - y\|_1$

subject to $Bx \leq 0$

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



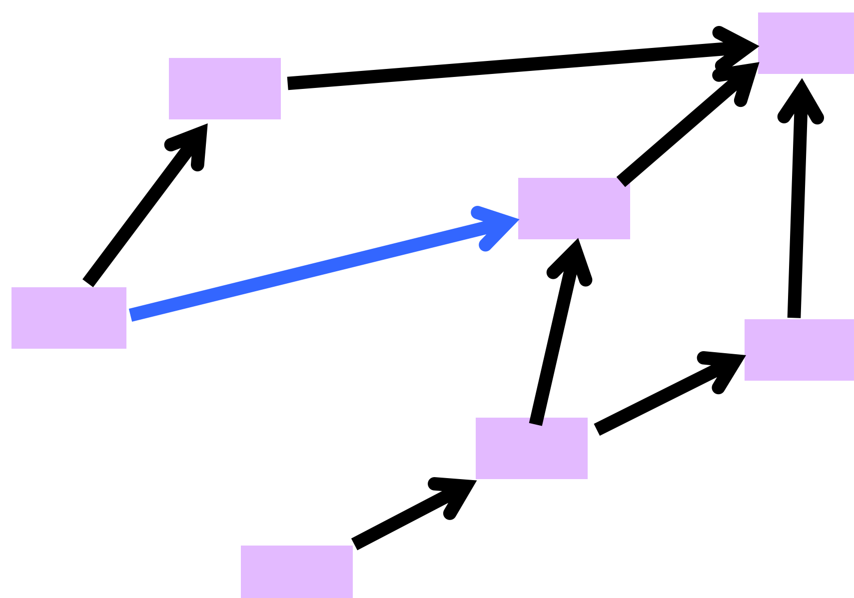
Linear Program for Isotonic Regression

Given y, minimize $\sum_i r_i$

subject to $Bx \leq 0$

$$|x_i - y_i| = r_i$$

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



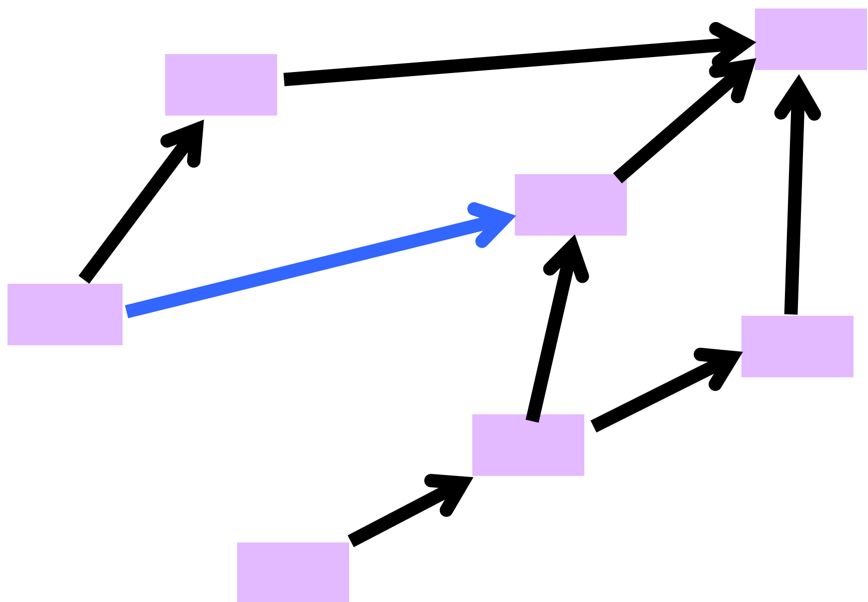
Linear Program for Isotonic Regression

Given y, minimize $\sum_i r_i$

subject to $Bx \leq 0$

$$|x_i - y_i| \leq r_i$$

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



Linear Program for Isotonic Regression

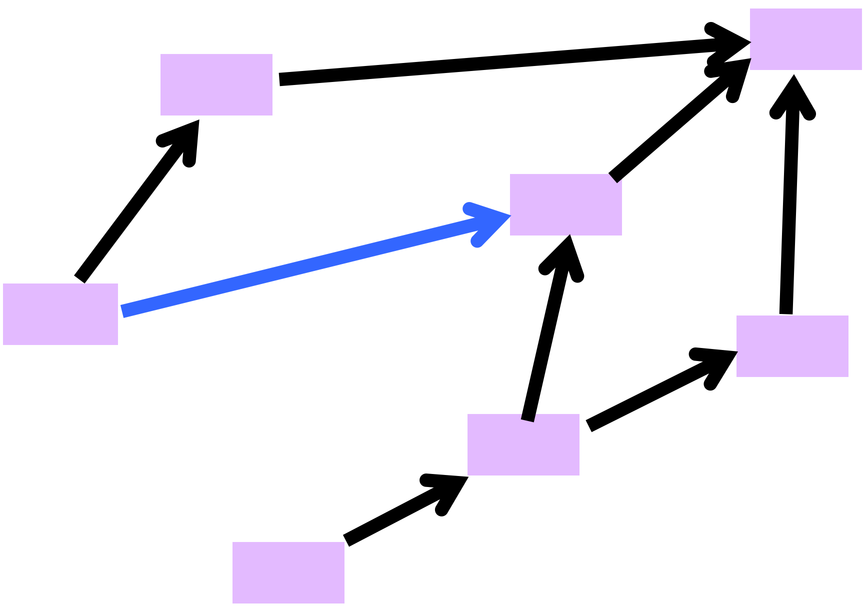
Given y, minimize $\sum_i r_i$

subject to $Bx \leq 0$

$$x_i - y_i \leq r_i$$

$$-(x_i - y_i) \leq r_i$$

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



Linear Program for Isotonic Regression

Minimize $\sum_i r_i$

subject to
$$\begin{pmatrix} 0 & B \\ -I & I \\ -I & -I \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} \leq \begin{pmatrix} 0 \\ y \\ -y \end{pmatrix}$$

Linear Program for Isotonic Regression

Minimize $\sum_i r_i$

subject to $\begin{pmatrix} 0 & B \\ -I & I \\ -I & -I \end{pmatrix} \begin{pmatrix} r \\ x \end{pmatrix} \leq \begin{pmatrix} 0 \\ y \\ -y \end{pmatrix}$

IPM solves a sequence of equations of form

$$\begin{pmatrix} 0 & B \\ -I & I \\ -I & -I \end{pmatrix}^T \begin{pmatrix} S_0 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_2 \end{pmatrix} \begin{pmatrix} 0 & B \\ -I & I \\ -I & -I \end{pmatrix}$$

with positive diagonal matrices S_0, S_1, S_2

Linear Program for Isotonic Regression

$$\begin{pmatrix} 0 & B \\ -I & I \\ -I & -I \end{pmatrix}^T \begin{pmatrix} S_0 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_2 \end{pmatrix} \begin{pmatrix} 0 & B \\ -I & I \\ -I & -I \end{pmatrix}$$

$$= \begin{pmatrix} S_1 + S_2 & S_2 - S_1 \\ S_2 - S_1 & \underbrace{B^T S_0 B}_{\text{Laplacian!}} + S_1 + S_2 \end{pmatrix}$$

S_0, S_1, S_2 are positive diagonal

Linear Program for Isotonic Regression

$$\begin{pmatrix} 0 & B \\ -I & I \\ -I & -I \end{pmatrix}^T \begin{pmatrix} S_0 & 0 & 0 \\ 0 & S_1 & 0 \\ 0 & 0 & S_2 \end{pmatrix} \begin{pmatrix} 0 & B \\ -I & I \\ -I & -I \end{pmatrix}$$

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S_0, S_1, S_2 are positive diagonal

Kyng, Rao, Sachdeva '15:
Reduce to solving Laplacians to constant accuracy

Spectral Sparsification

Every graph can be approximated
by a sparse graph with a similar Laplacian

Approximating Graphs

A graph H is an ϵ-approximation of G if

for all x $$\frac{1}{1+\epsilon} \leq \frac{x^T L_H x}{x^T L_G x} \leq 1+\epsilon$$

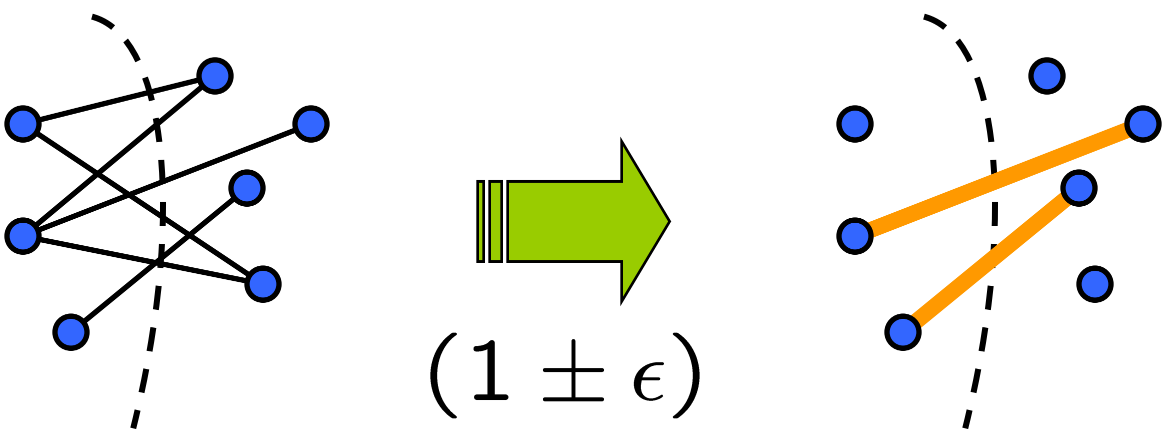
$$L_H \approx_\epsilon L_G$$

Approximating Graphs

A graph H is an ϵ-approximation of G if

for all x
$$\frac{1}{1+\epsilon} \leq \frac{x^T L_H x}{x^T L_G x} \leq 1+\epsilon$$

Preserves boundaries of every set



Approximating Graphs

A graph H is an ϵ-approximation of G if

for all x $$\frac{1}{1+\epsilon} \leq \frac{x^T L_H x}{x^T L_G x} \leq 1+\epsilon$$

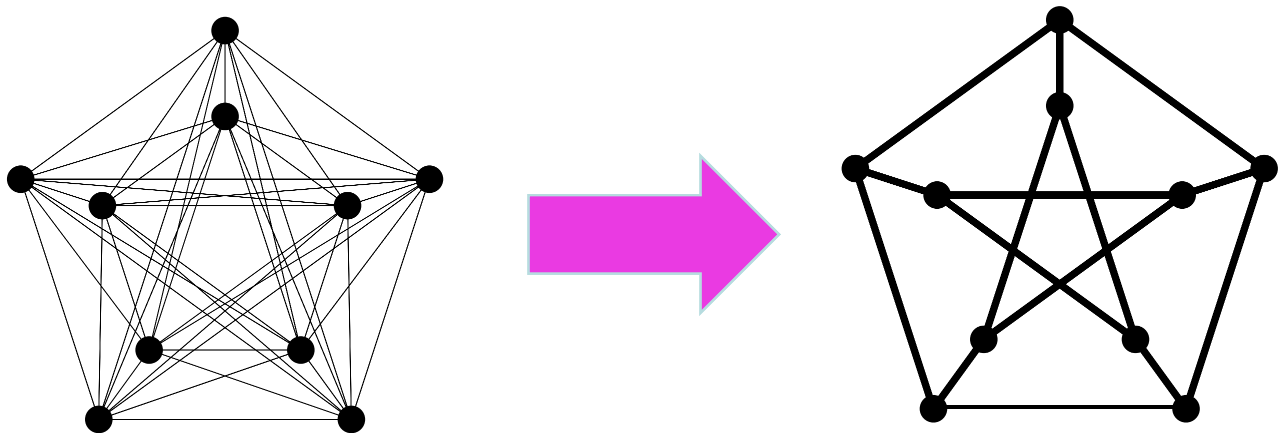
Solutions to linear equations are similiar

$$L_H \approx_\epsilon L_G \iff L_H^{-1} \approx_\epsilon L_G^{-1}$$

Spectral Sparsification

(Batson, S, Srivastava '09)

Every graph G has an ϵ-approximation H with $n(2+\epsilon)^2/\epsilon^2$ edges



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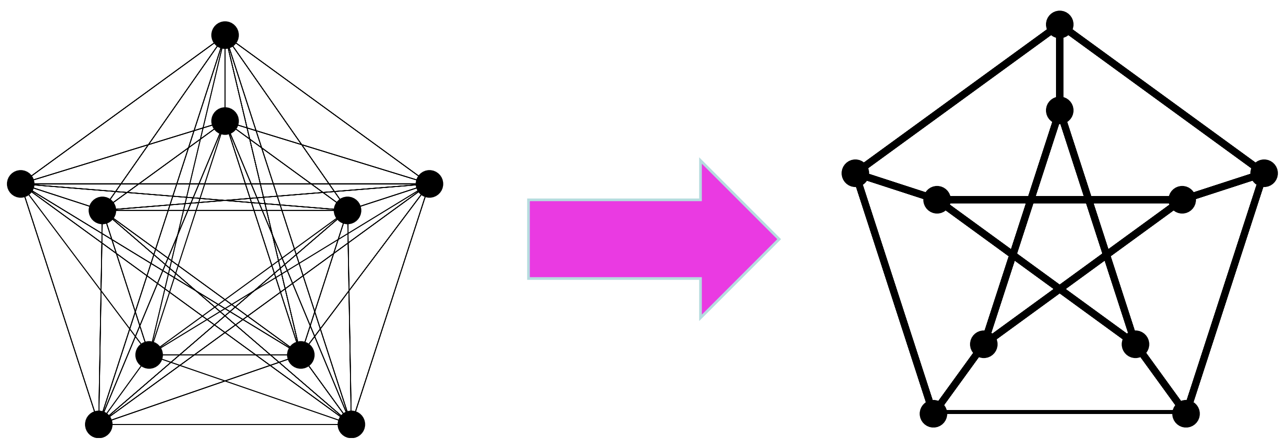

Random regular graphs approximate complete graphs

Fast Spectral Sparsification

(S & Srivastava '08)

If sample each edge with probability inversely proportional to its effective spring constant, only need $O(n \log n / \epsilon^2)$ samples

Takes time $O(m \log^2 n)$ (Koutis, Levin, Peng '12)

(Lee & Sun '15)

Can find an ϵ-approximation with $O(n/\epsilon^2)$ edges in time $O(n^{1+c})$ for every $c > 0$

Approximate Gaussian Elimination

(Kyng & Sachdeva '16)

Gaussian Elimination:

compute upper triangular U so that

$$L_G = U^T U$$

Approximate Gaussian Elimination:

compute sparse upper triangular U so that

$$L_G \approx U^T U$$

Gaussian Elimination

$$\begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 14 & 0 \\ -4 & -1 & 0 & 7 \end{pmatrix}$$

1. Find the rank-1 matrix that agrees on the first row and column

$$\begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 1 & 2 & 1 \\ -8 & 2 & 4 & 2 \\ -4 & 1 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 4 \\ -1 \\ -2 \\ -1 \end{pmatrix} \begin{pmatrix} 4 & -1 & -2 & -1 \end{pmatrix}$$

2. Subtract it

Gaussian Elimination

1. Find the rank-1 matrix that agrees on the first row and column

$$\begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 1 & 2 & 1 \\ -8 & 2 & 4 & 2 \\ -4 & 1 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 4 \\ -1 \\ -2 \\ -1 \end{pmatrix} \begin{pmatrix} 4 & -1 & -2 & -1 \end{pmatrix}$$

2. Subtract it

$$\begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 14 & 0 \\ -4 & -1 & 0 & 7 \end{pmatrix} - \begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 1 & 2 & 1 \\ -8 & 2 & 4 & 2 \\ -4 & 1 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 4 & -2 & -2 \\ 0 & -2 & 10 & -2 \\ 0 & -2 & -2 & 6 \end{pmatrix}$$

3. Repeat

Gaussian Elimination

2. Subtract it

$$\begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 14 & 0 \\ -4 & -1 & 0 & 7 \end{pmatrix} - \begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 1 & 2 & 1 \\ -8 & 2 & 4 & 2 \\ -4 & 1 & 2 & 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 4 & -2 & -2 \\ 0 & -2 & 10 & -2 \\ 0 & -2 & -2 & 6 \end{pmatrix}$$

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Gaussian Elimination

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Gaussian Elimination

$$\begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 14 & 0 \\ -4 & -1 & 0 & 7 \end{pmatrix}$$

$$= \begin{pmatrix} 4 \\ -1 \\ -2 \\ -1 \end{pmatrix} \begin{pmatrix} 4 \\ -1 \\ -2 \\ -1 \end{pmatrix}^T + \begin{pmatrix} 0 \\ 2 \\ -1 \\ -1 \end{pmatrix} \begin{pmatrix} 0 \\ 2 \\ -1 \\ -1 \end{pmatrix}^T + \begin{pmatrix} 0 \\ 0 \\ 3 \\ -1 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 3 \\ -1 \end{pmatrix}^T + \begin{pmatrix} 0 \\ 0 \\ 0 \\ 2 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 2 \end{pmatrix}^T$$

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$$= \begin{pmatrix} 4 & 0 & 0 & 0 \\ -1 & 2 & 0 & 0 \\ -2 & -1 & 3 & 0 \\ -1 & -1 & -1 & 2 \end{pmatrix} \begin{pmatrix} 4 & -1 & -2 & -1 \\ 0 & 2 & -1 & -1 \\ 0 & 0 & 3 & -1 \\ 0 & 0 & 0 & 2 \end{pmatrix}$$

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Computation time proportional to the sum of the squares of the number of nonzeros in these vectors

Gaussian Elimination of Laplacians

If this is a Laplacian, then so is this

$$\begin{pmatrix} 16 & -4 & -8 & -4 \\ -4 & 5 & 0 & -1 \\ -8 & 0 & 14 & 0 \\ -4 & -1 & 0 & 7 \end{pmatrix} - \begin{pmatrix} 4 \\ -1 \\ -2 \\ -1 \end{pmatrix} \begin{pmatrix} 4 \\ -1 \\ -2 \\ -1 \end{pmatrix}^T = \begin{pmatrix} 0 & 0 & 0 & 0 \\ 0 & 4 & -2 & -2 \\ 0 & -2 & 10 & -2 \\ 0 & -2 & -2 & 6 \end{pmatrix}$$

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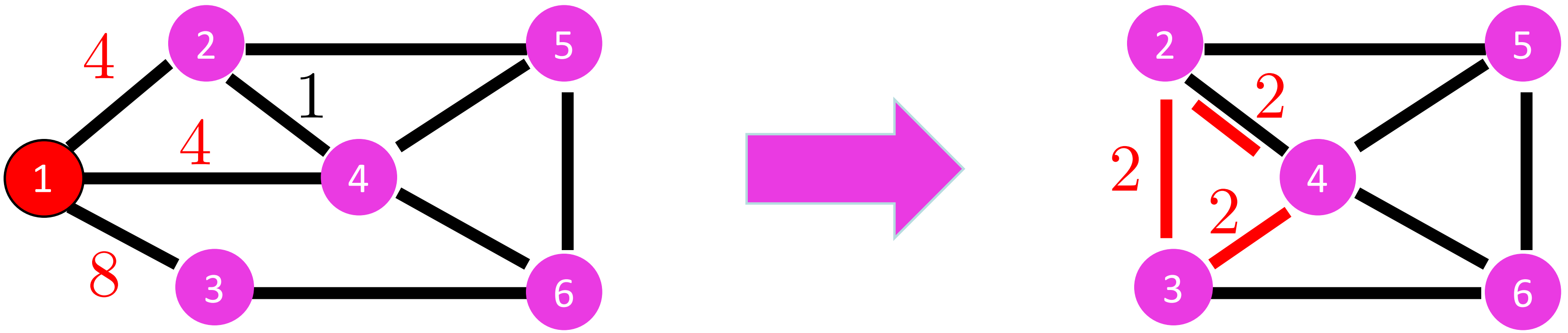
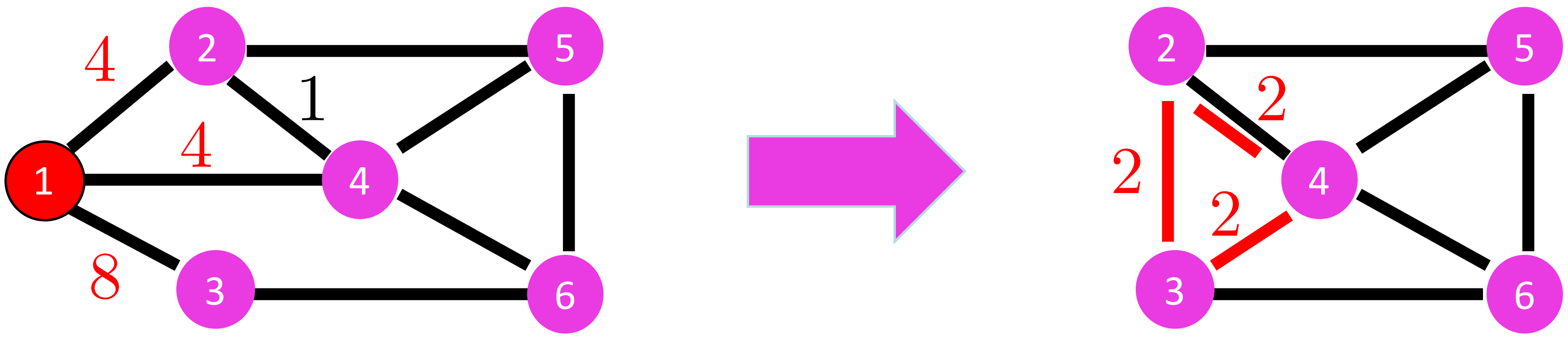
When eliminate a node, add a clique on its neighbors



Approximate Gaussian Elimination

(Kyng & Sachdeva '16)

1. when eliminate a node, add a clique on its neighbors



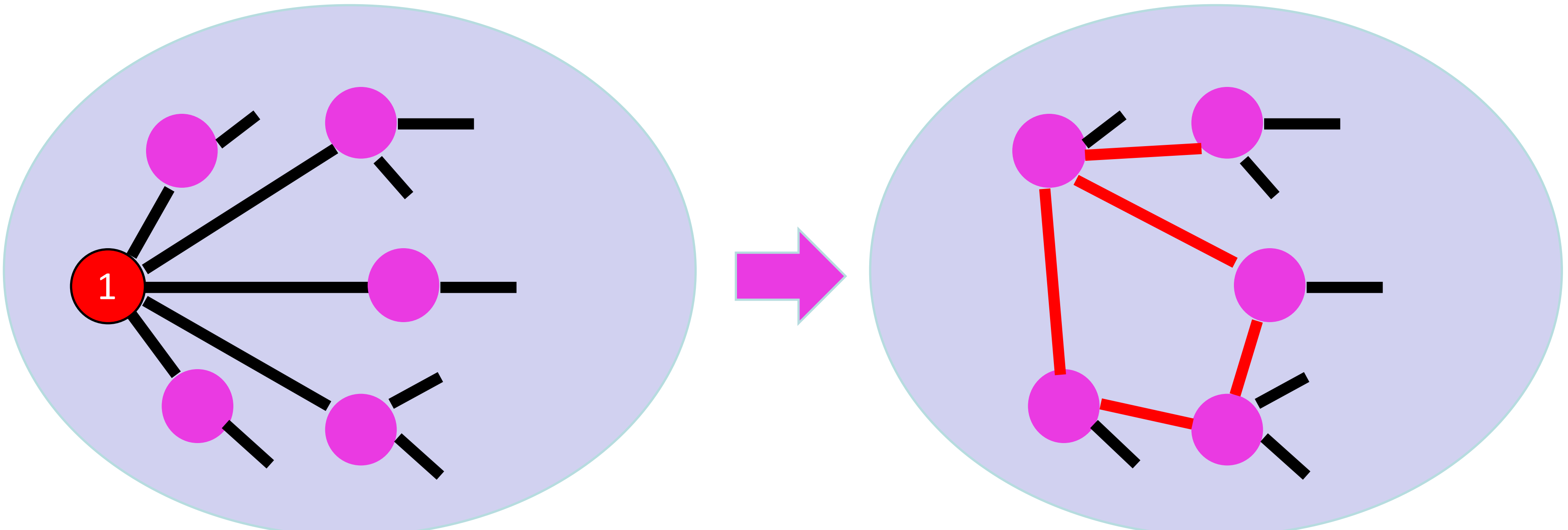
2. Sparsify that clique, without ever constructing it

Approximate Gaussian Elimination

(Kyng & Sachdeva '16)

1. When eliminate a node of degree d,

   add d edges at random between its neighbors, sampled with probability proportional to the weight of the edge to the eliminated node



Approximate Gaussian Elimination

(Kyng & Sachdeva '16)

0. Initialize by randomly permuting vertices, and making $O(\log^2 n)$ copies of every edge

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Total time is $O(m \log^3 n)$

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Total time is $O(m \log^3 n)$

Can be improved by sacrificing some simplicity

Approximate Gaussian Elimination

(Kyng & Sachdeva '16)

Analysis by Random Matrix Theory:

Write $U^T U$ as a sum of random matrices.

$$\mathbb{E}\left[U^T U\right] = L_G$$

Random permutation and copying
control the variances of the random matrices

Apply Matrix Freedman inequality (Tropp '11)

Recent Developments

Other families of linear systems

(Kyng, Lee, Peng, Sachdeva, S '16)

complex-weighted Laplacians $\begin{pmatrix} 1 & e^{i\theta} \\ e^{-i\theta} & 1 \end{pmatrix}$

connection Laplacians $\begin{pmatrix} I & Q \\ Q^T & I \end{pmatrix}$

Laplacians.jl

To learn more

My web page on:

Laplacian linear equations, sparsification, local graph clustering, low-stretch spanning trees, and so on.

My class notes from

"Graphs and Networks" and "Spectral Graph Theory"

$Lx = b$, by Nisheeth Vishnoi