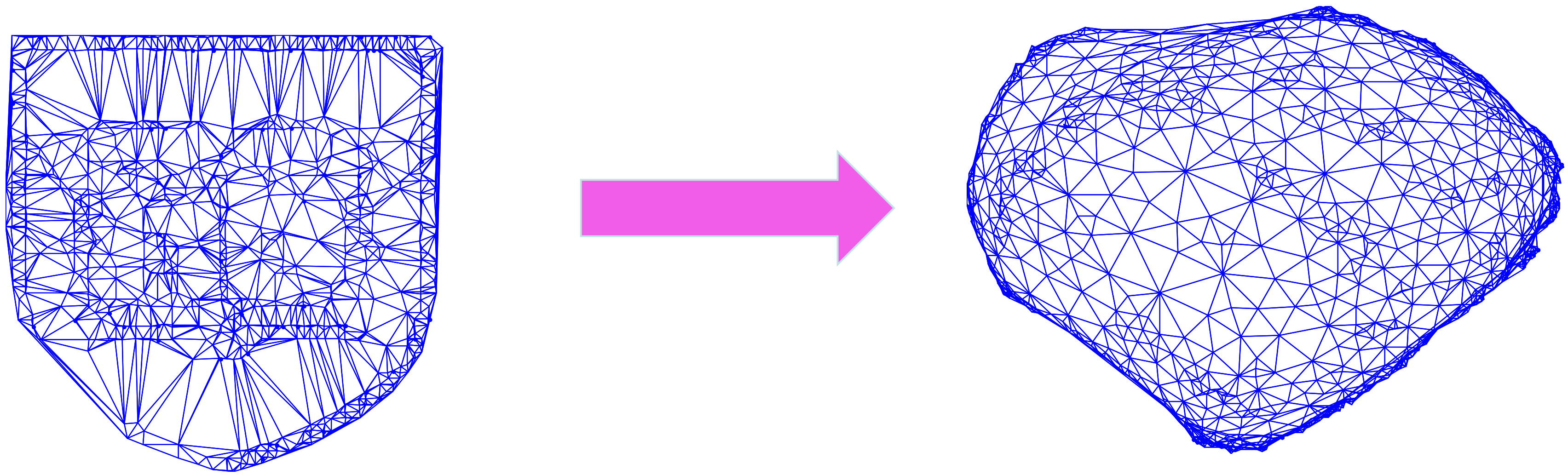
Laplacian Matrices of Graphs:
Spectral and Electrical Theory



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Toronto, Sep. 28, 2011

Outline

Introduction to graphs

Physical metaphors

Laplacian matrices

Spectral graph theory

A very fast survey

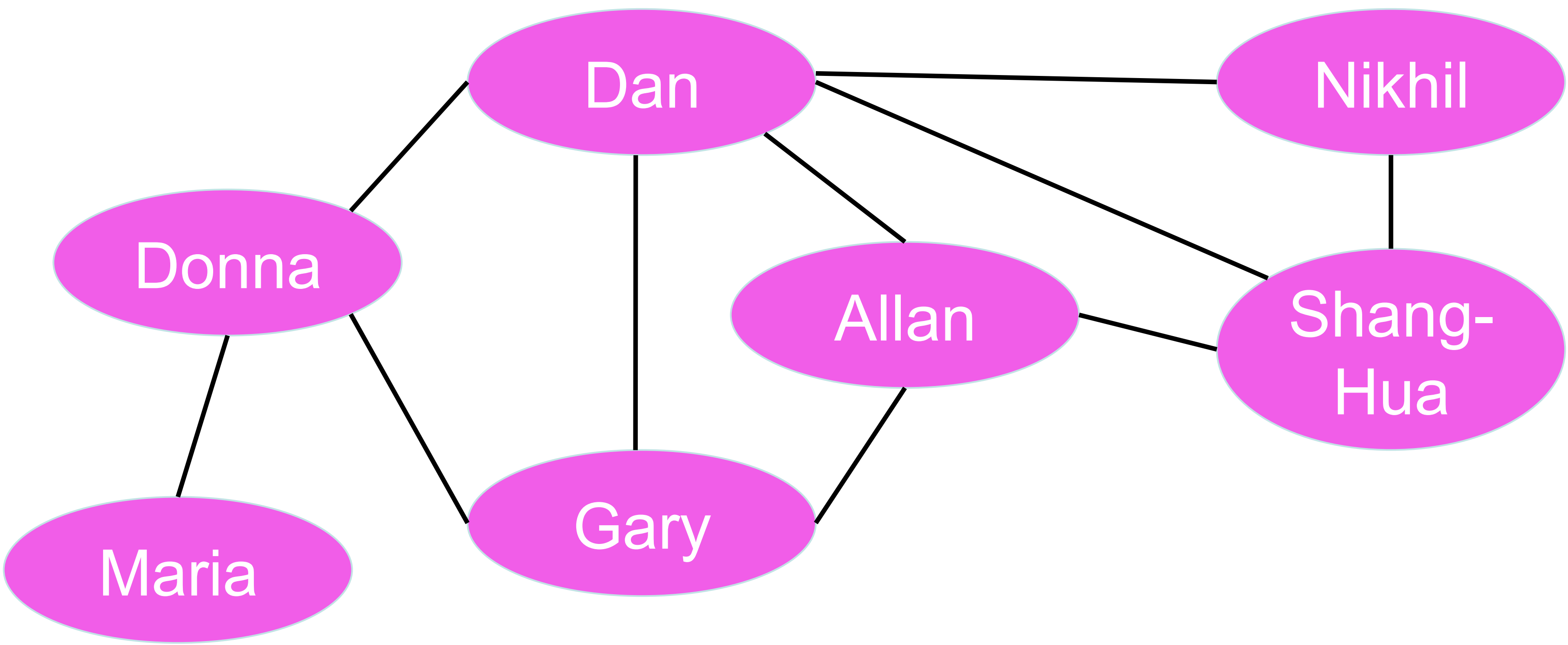
Trailer for lectures 2 and 3

Graphs and Networks

V: a set of vertices (nodes)

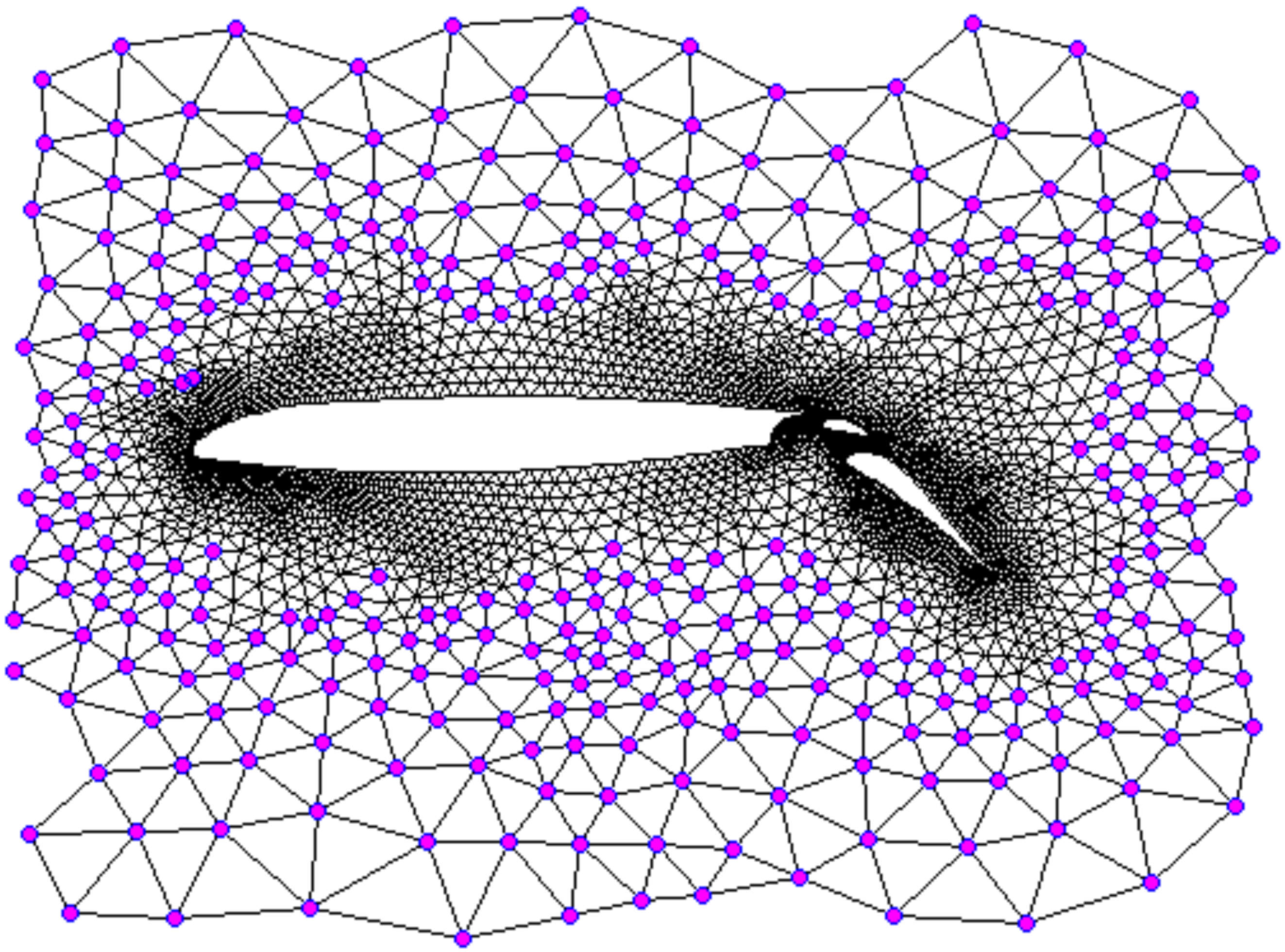
E: a set of edges

an edge is a pair of vertices



Difficult to draw when big

Examples of Graphs



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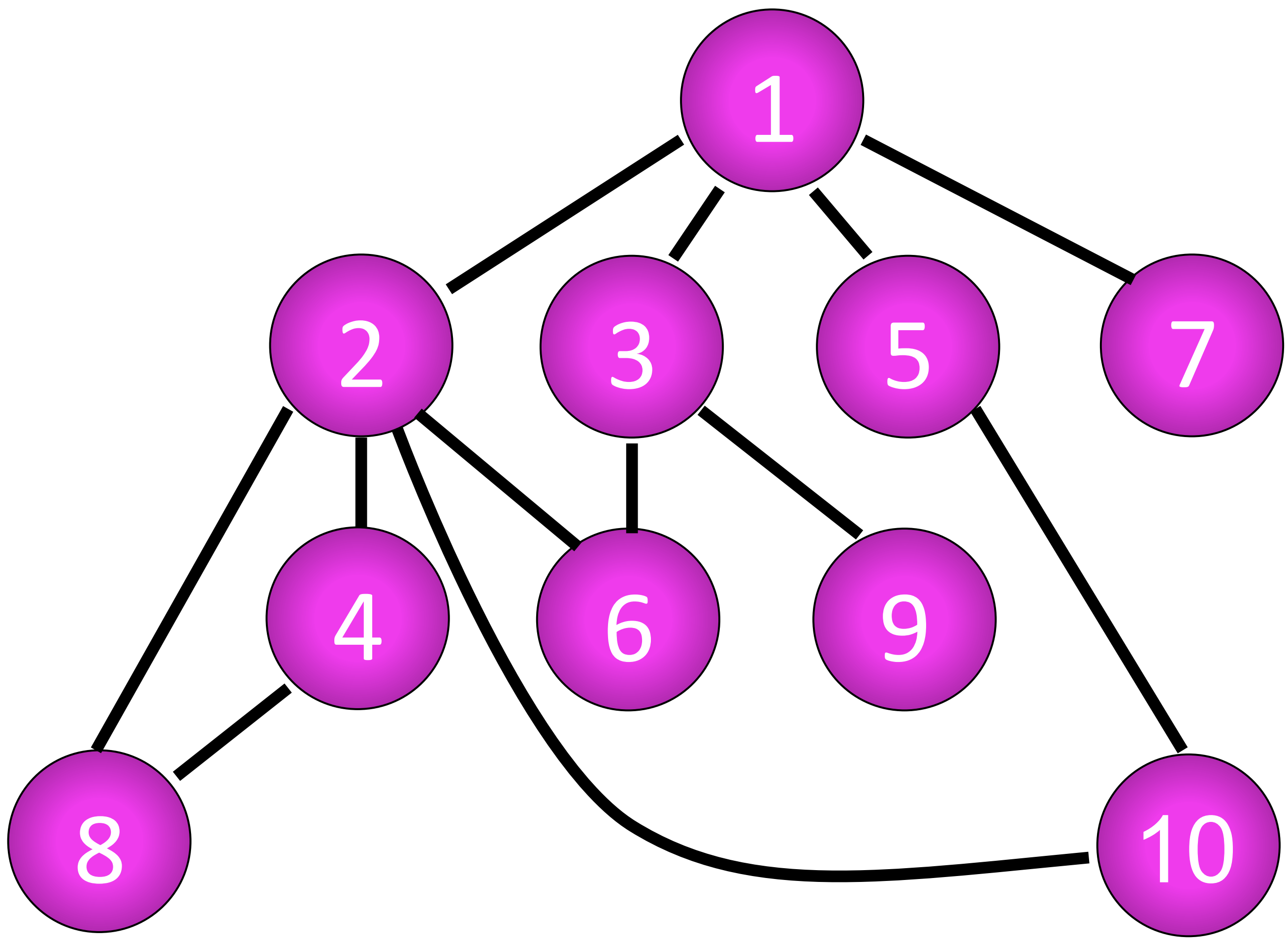

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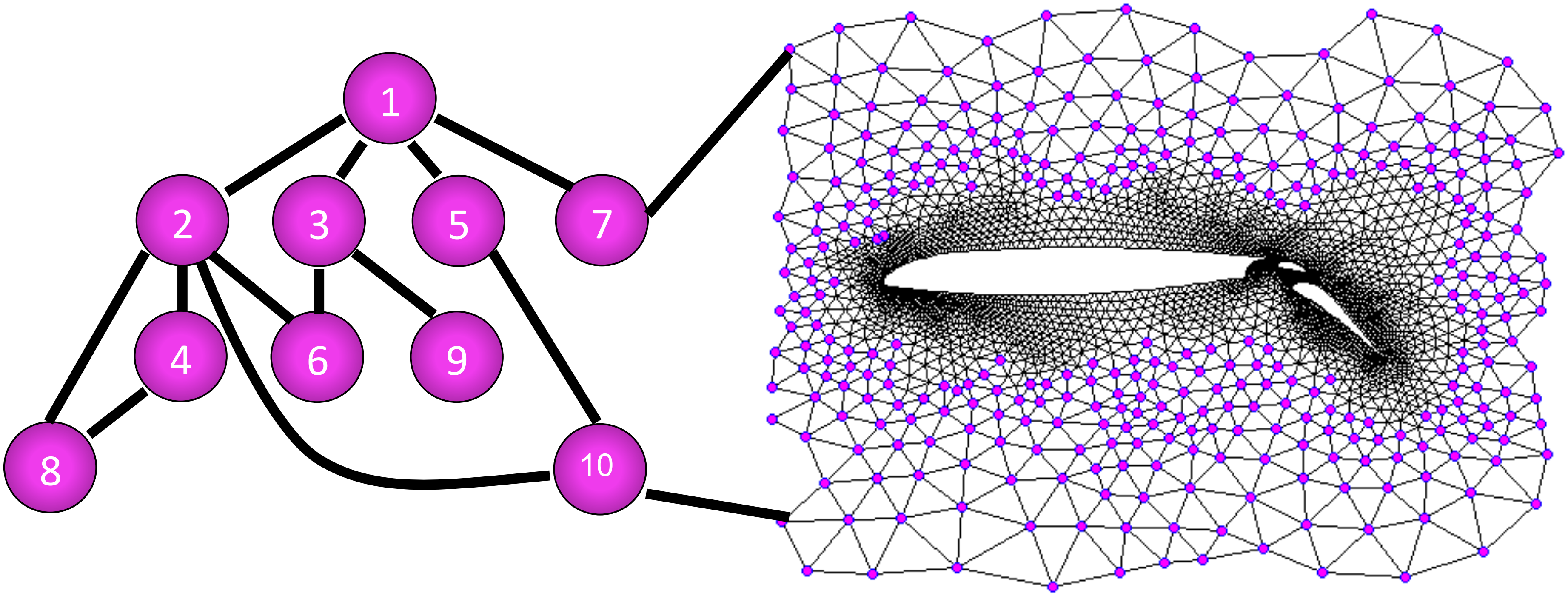

How to understand a graph

Use physical metaphors
- Edges as rubber bands
- Edges as resistors

Examine processes
- Diffusion of gas
- Spilling paint

Identify structures
- Communities

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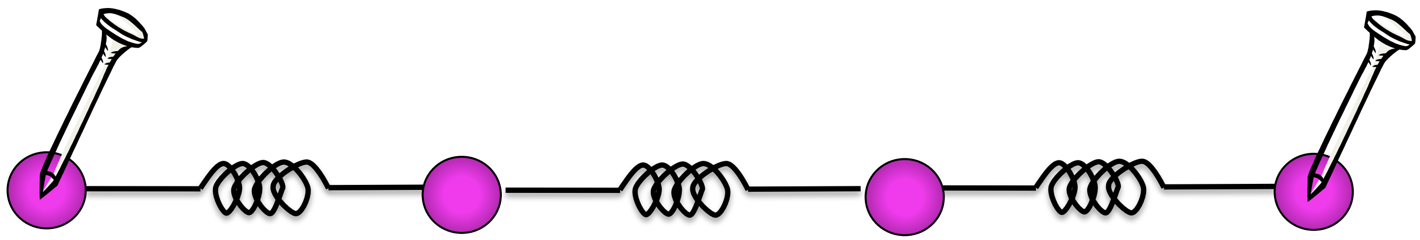
Graphs as Spring Networks

View edges as rubber bands or ideal linear springs
spring constant 1 (for now)

Nail down some vertices, let rest settle



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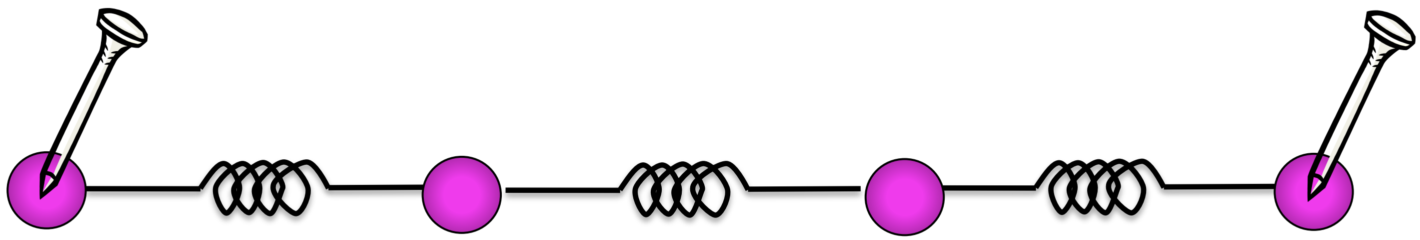

When stretched to length ℓ

potential energy is $\ell^2/2$

Graphs as Spring Networks

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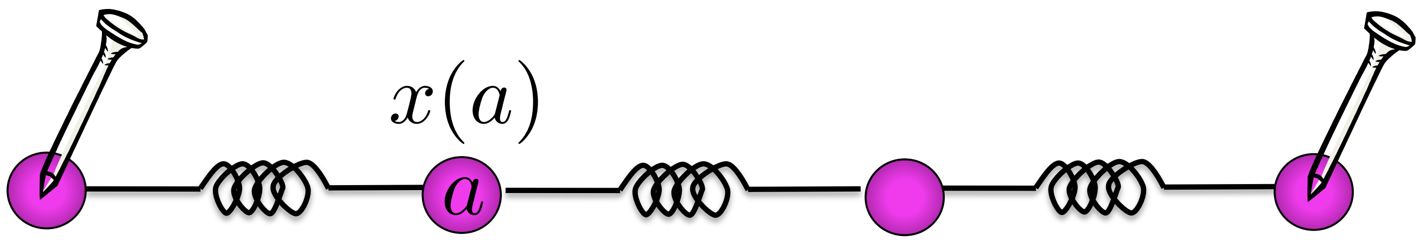


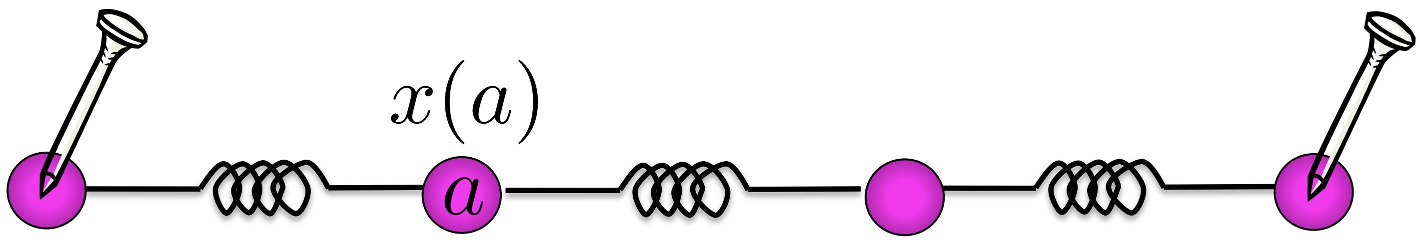
Physics: position minimizes total potential energy

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

subject to boundary constraints (nails)

Graphs as Spring Networks

Nail down some vertices, let rest settle



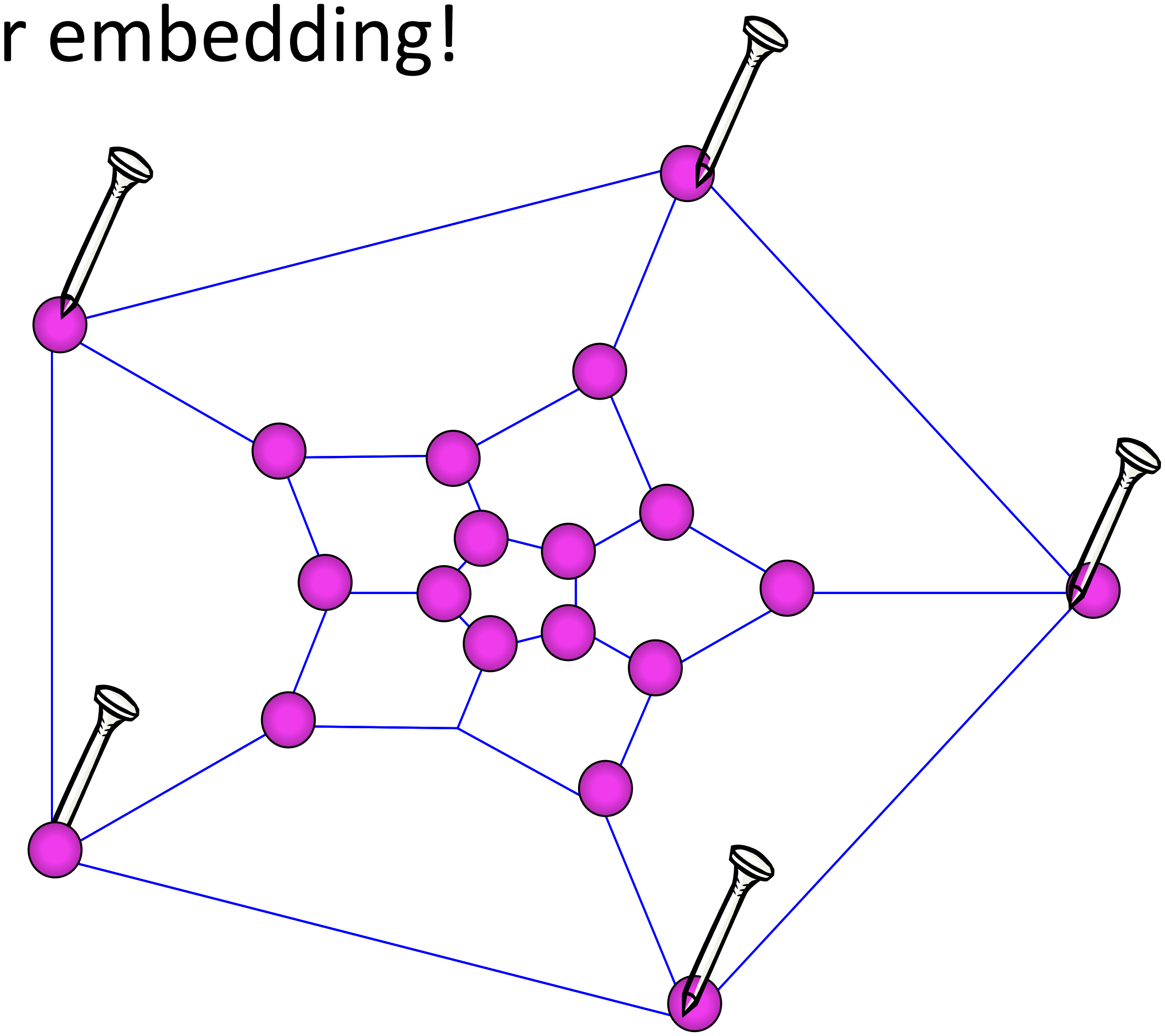
Energy minimized when
free vertices are averages of neighbors

$$\vec{x}(a) = \frac{1}{d_a} \sum_{(a,b)\in E} \vec{x}(b)$$

d_a is *degree* of a, number of attached edges

Tutte's Theorem '63

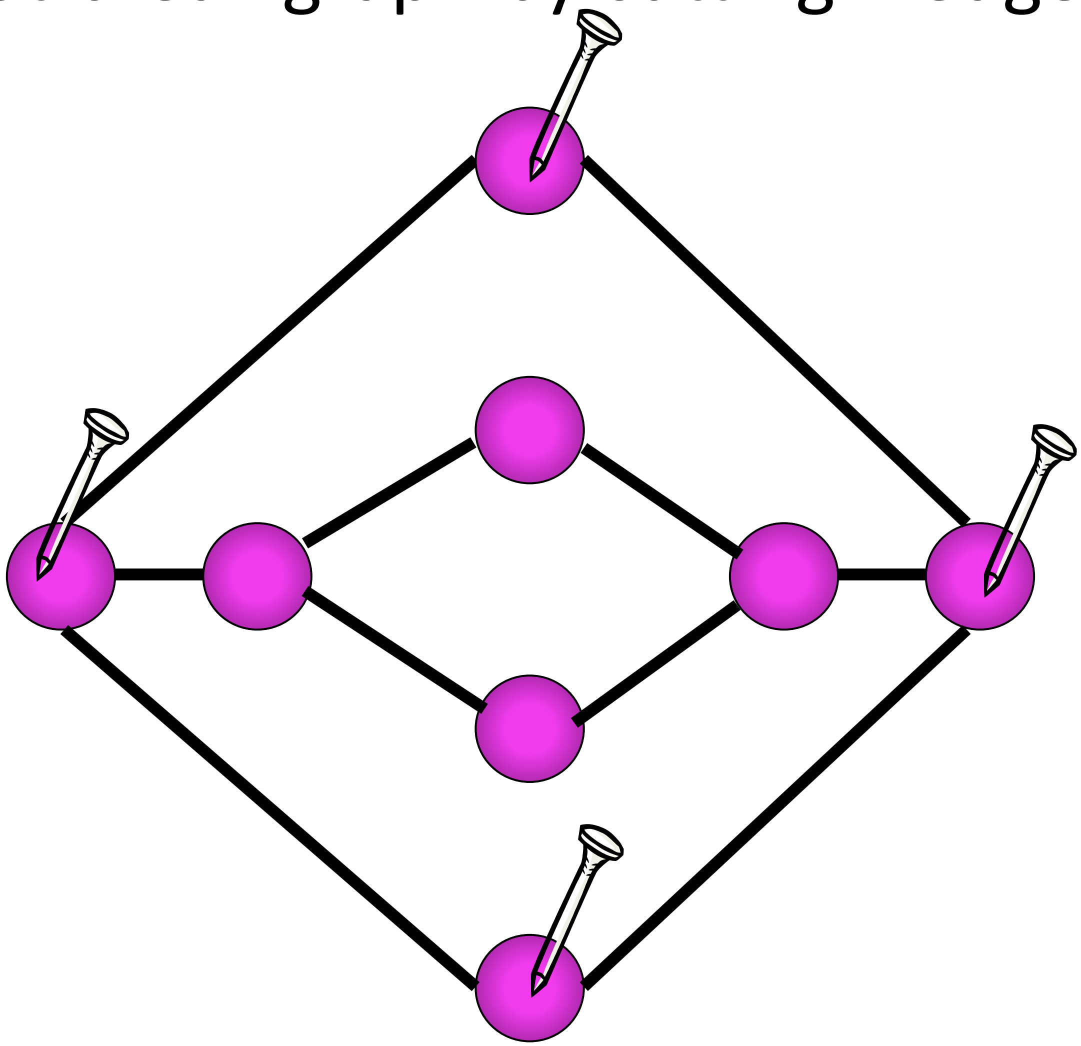
If nail down a face of a planar 3-connected graph, get a planar embedding!



Tutte's Theorem '63

3-connected:

cannot break graph by cutting 2 edges



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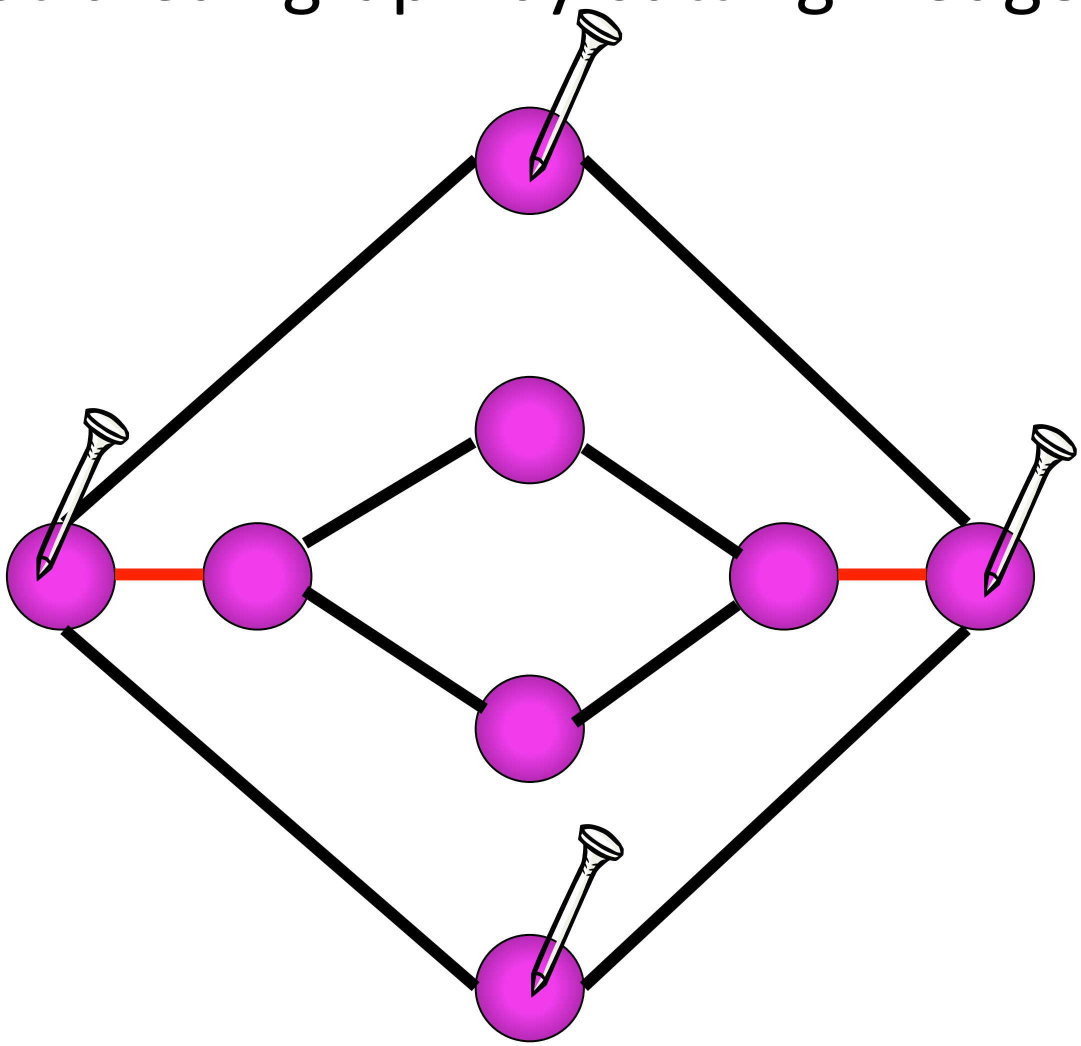

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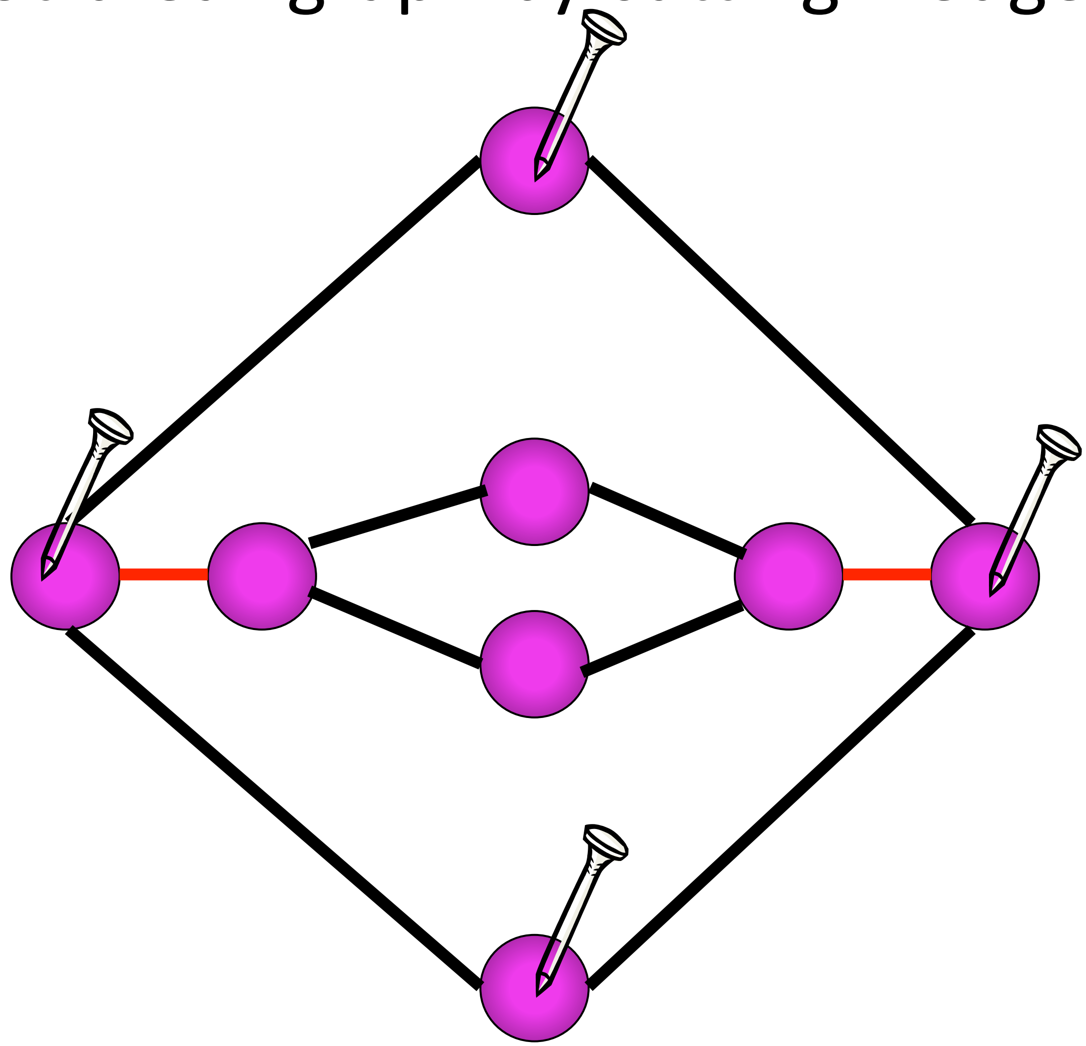

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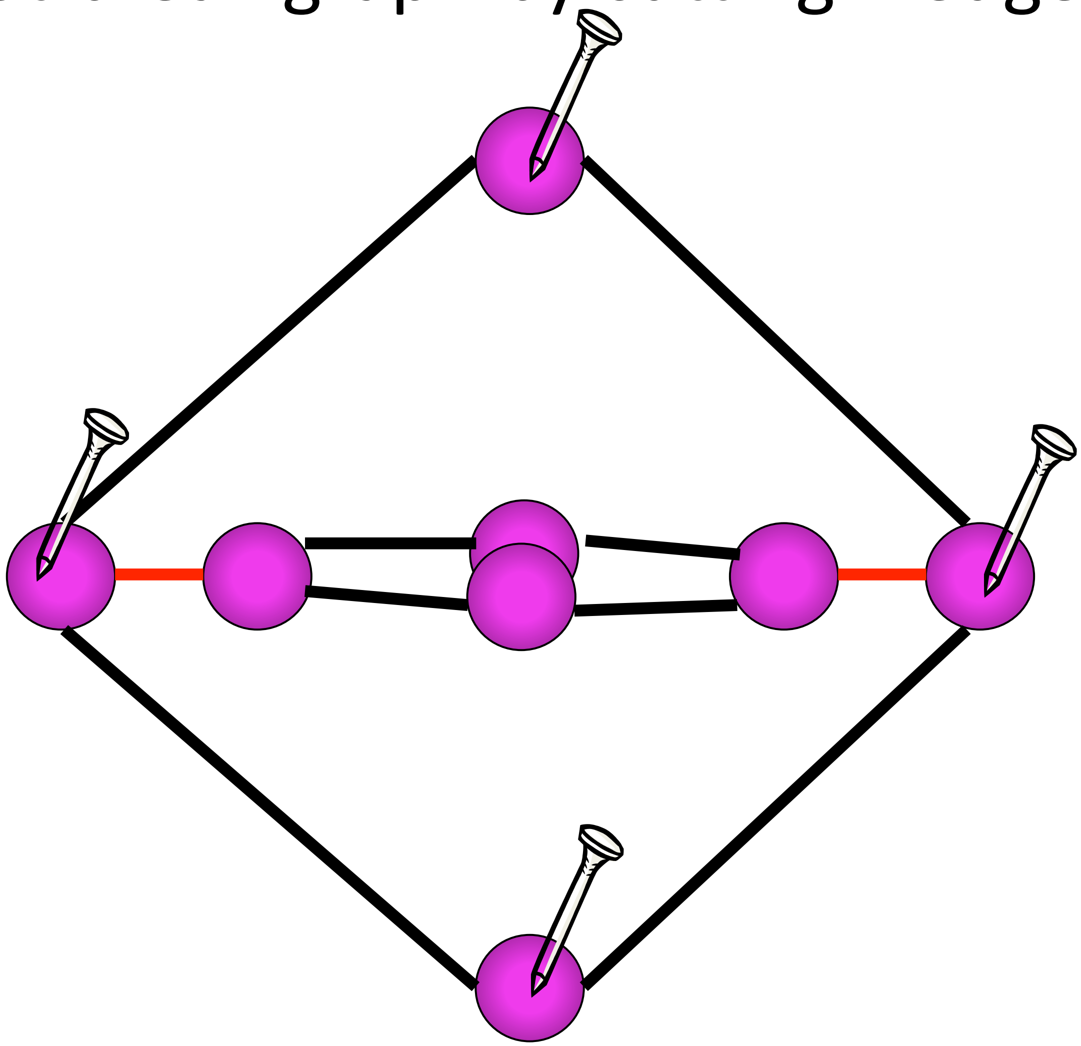
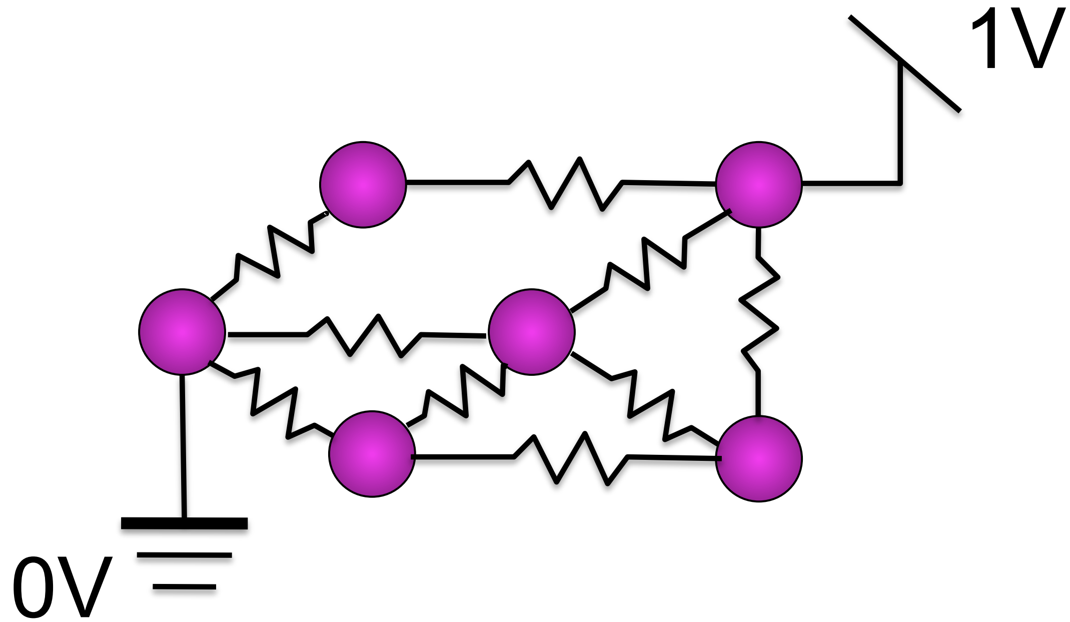


Graphs as Resistor Networks

View edges as resistors connecting vertices

Apply voltages at some vertices.
Measure induced voltages and current flow.



Graphs as Resistor Networks

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Current flow measures strength of connection between endpoints.

More short disjoint paths lead to higher flow.

Graphs as Resistor Networks

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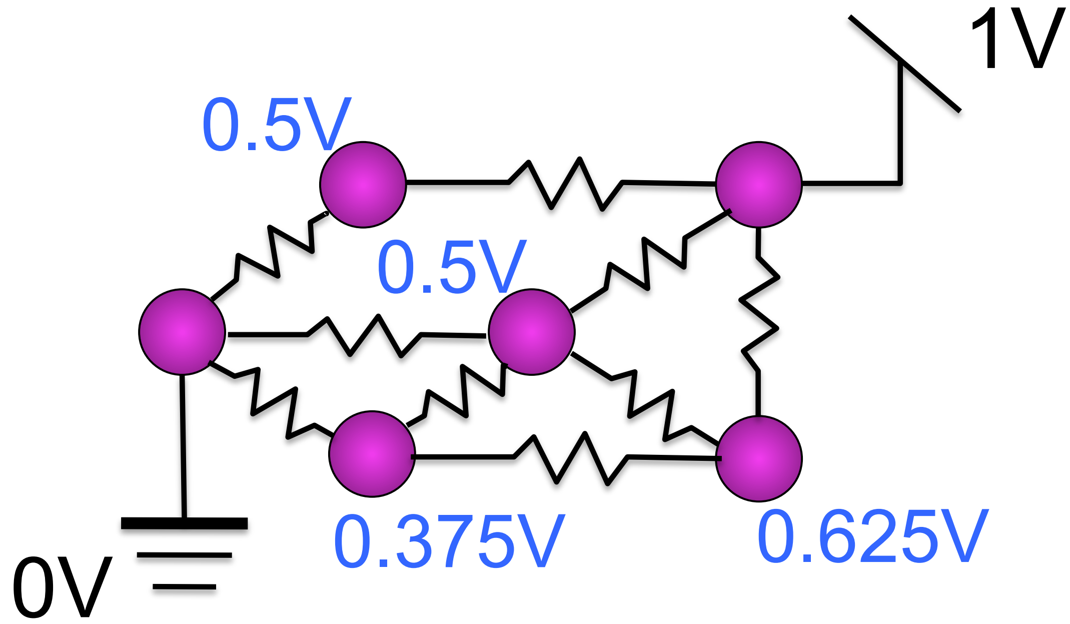


Graphs as Resistor Networks

View edges as resistors connecting vertices

Apply voltages at some vertices.
Measure induced voltages and current flow.

Induced voltages minimize

$$\sum_{(a,b)\in E} (v(a) - v(b))^2$$

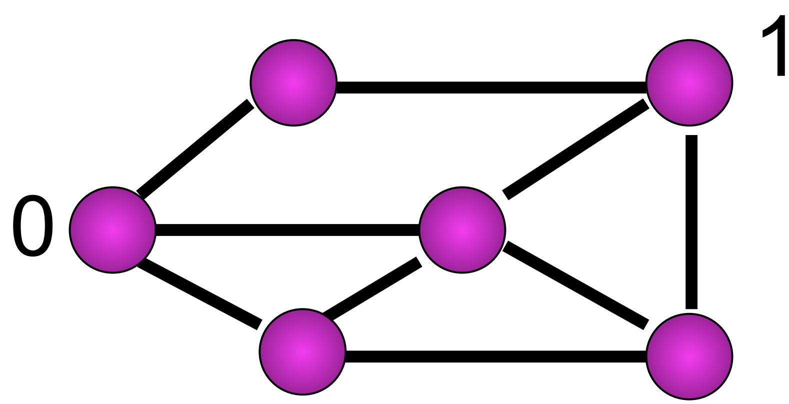
Subject to fixed voltages (by battery)

Learning on Graphs [Zhu-Ghahramani-Lafferty '03]

Infer values of a function at all vertices
from known values at a few vertices.

Minimize $$\sum_{(a,b)\in E} (x(a) - x(b))^2$$

Subject to known values



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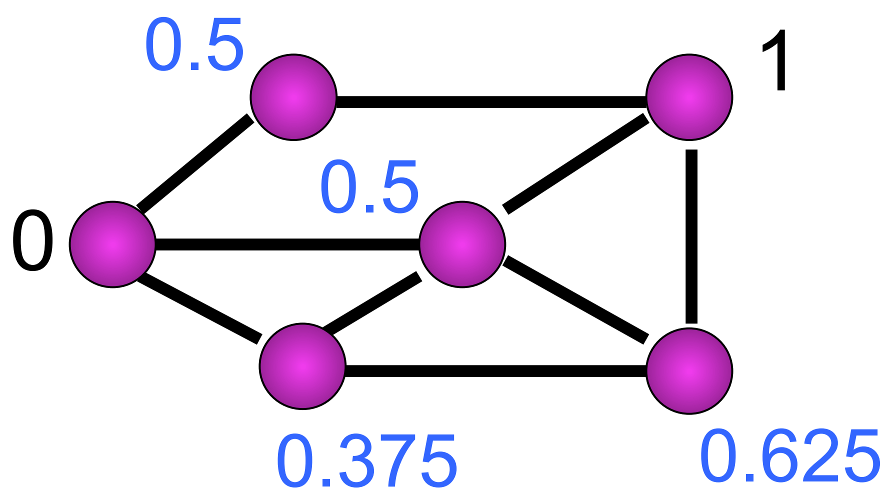

The Laplacian quadratic form

$$\sum_{(a,b)\in E} (x(a) - x(b))^2$$

The Laplacian matrix of a graph

$$x^T \underline{L} x = \sum_{(a,b)\in E} (x(a) - x(b))^2$$

The Laplacian matrix of a graph

$$x^T \underline{L} x = \sum_{(a,b) \in E} (x(a) - x(b))^2$$

To minimize subject to boundary constraints,
set derivative to zero.

Solve equation of form

$$Lx = b$$

Weighted Graphs

Edge (a, b) assigned a non-negative real weight
$w_{a,b} \in \mathbb{R}$ measuring
strength of connection
spring constant
1/resistance

$$x^T L x = \sum_{(a,b) \in E} w_{a,b} (x(a) - x(b))^2$$

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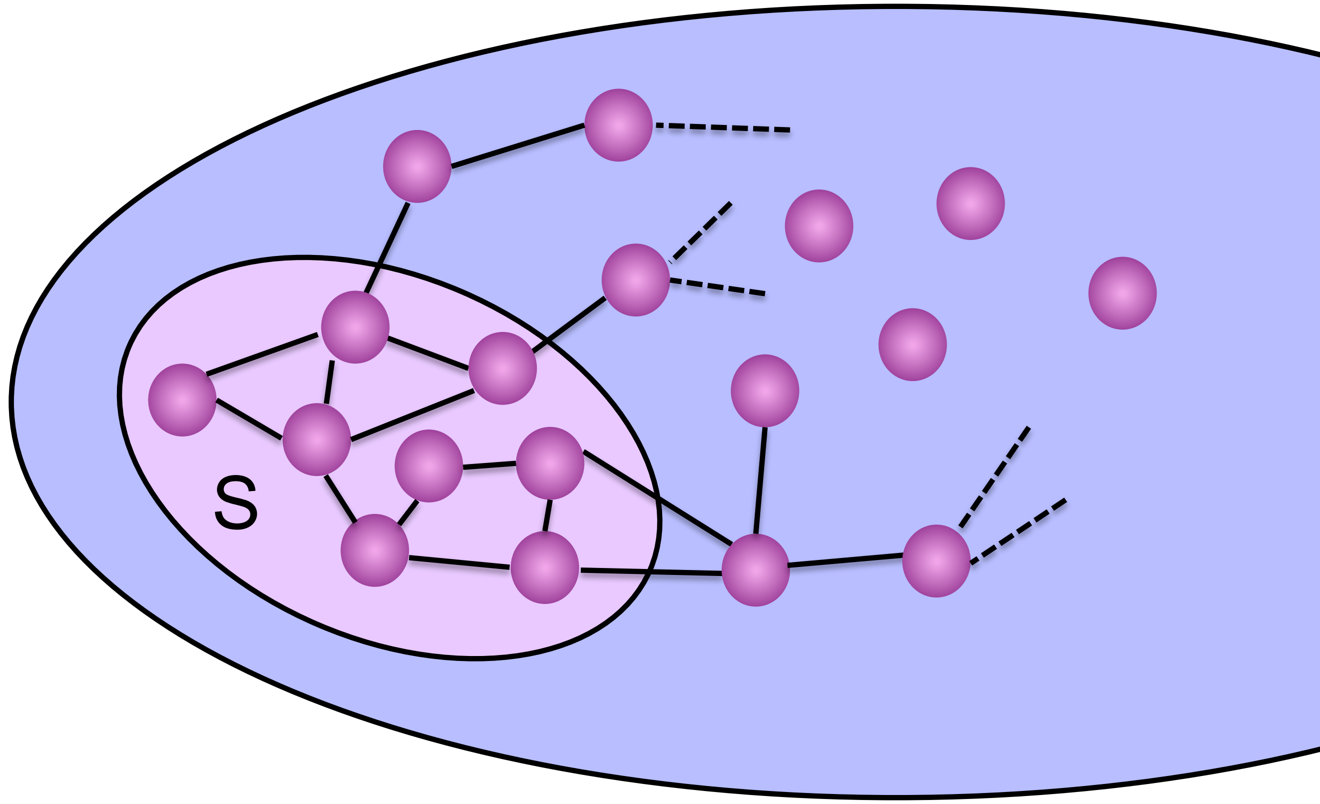
I'll show the matrix entries tomorrow

Measuring boundaries of sets

Boundary: edges leaving a set



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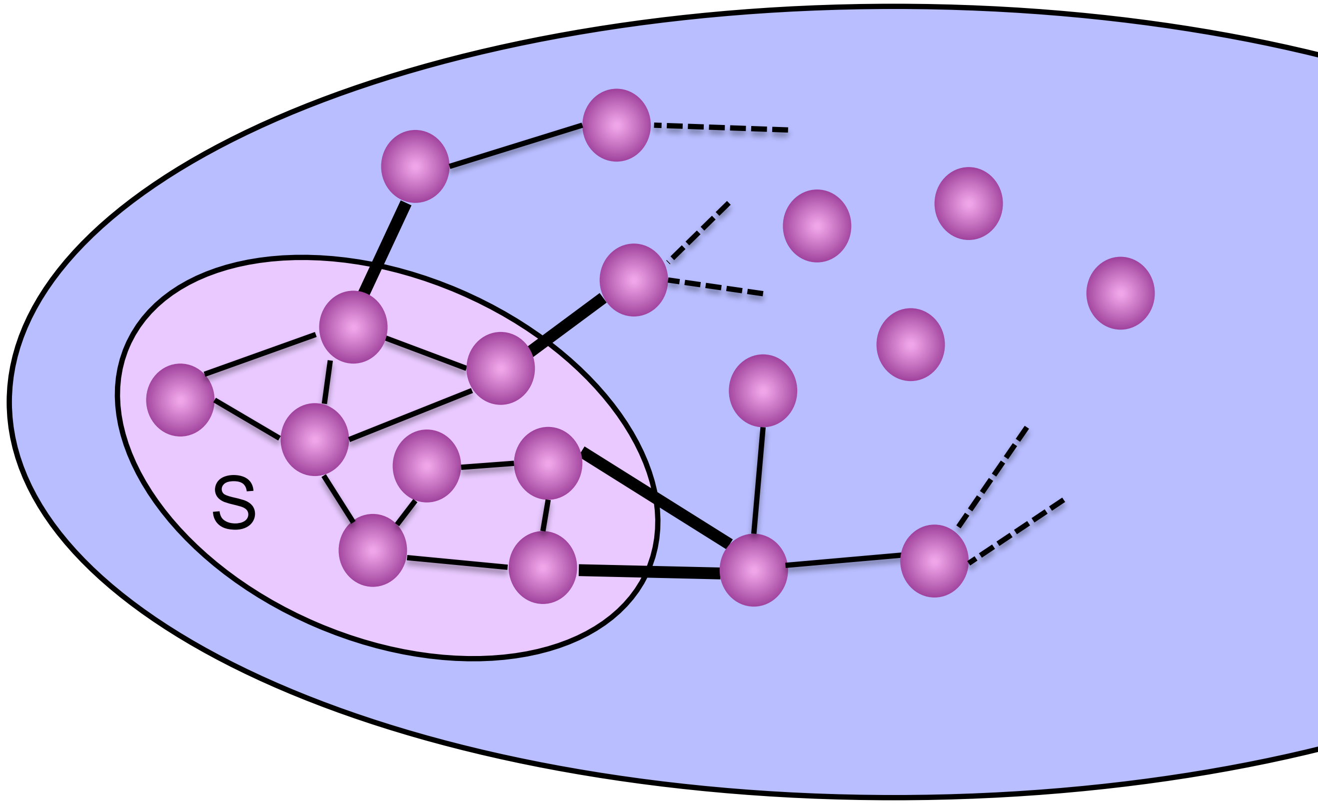
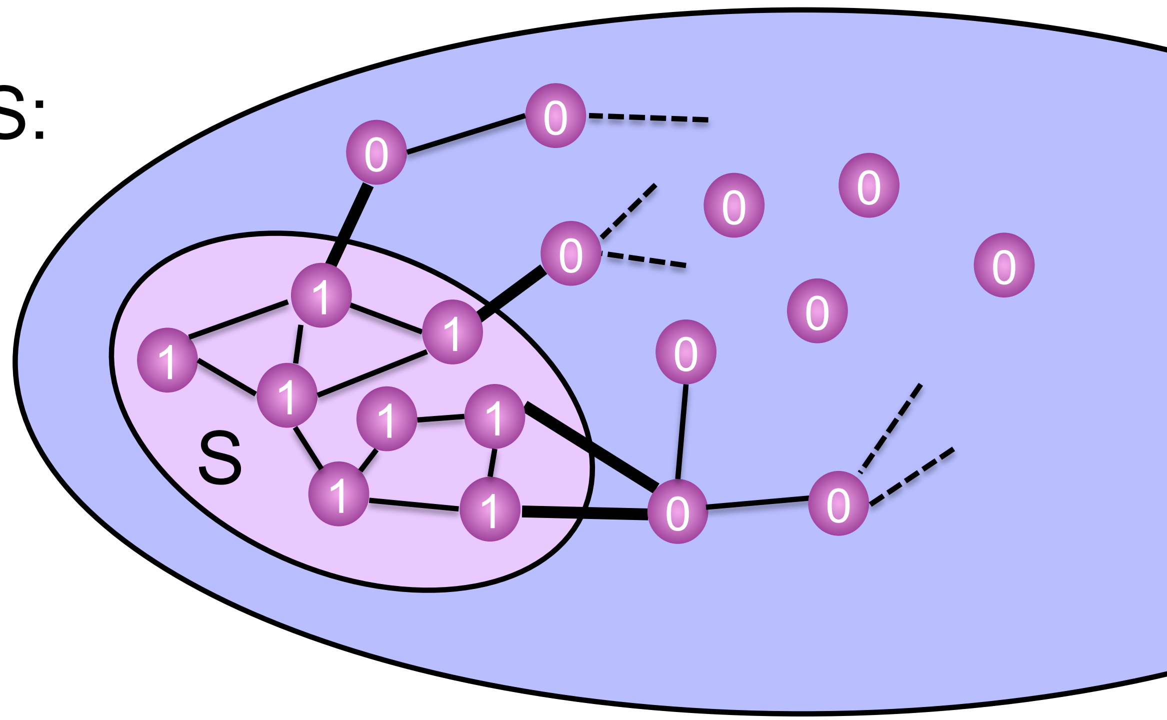


Measuring boundaries of sets

Boundary: edges leaving a set

Characteristic Vector of S:

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



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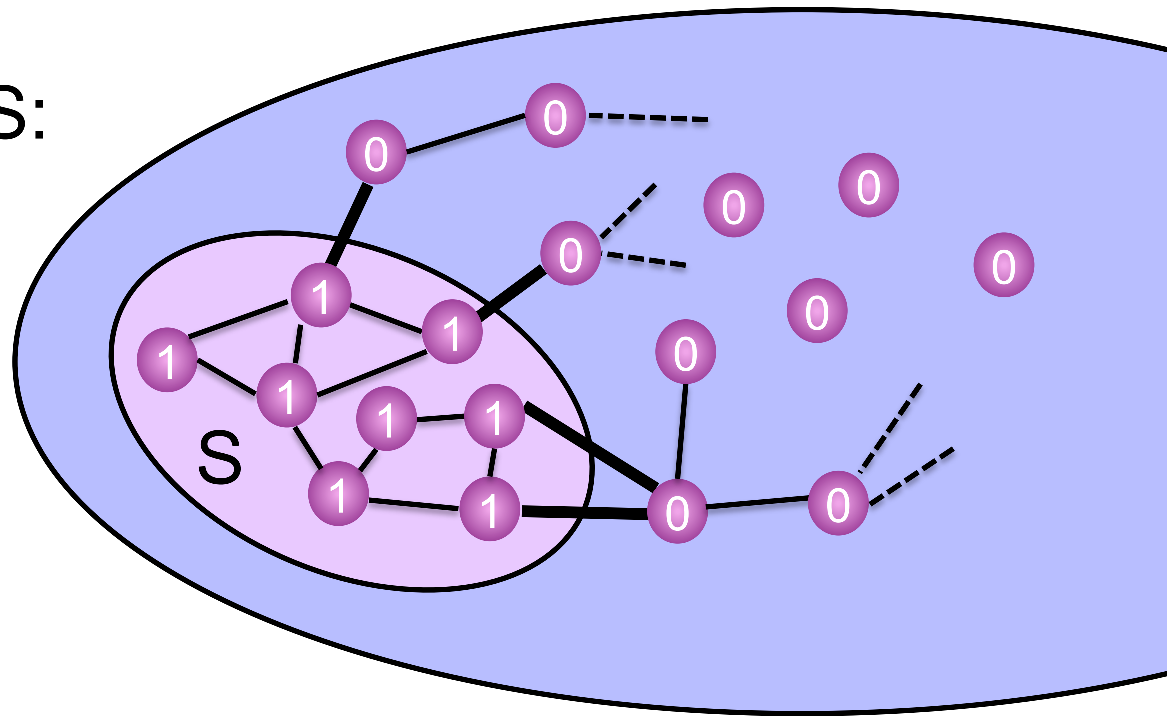


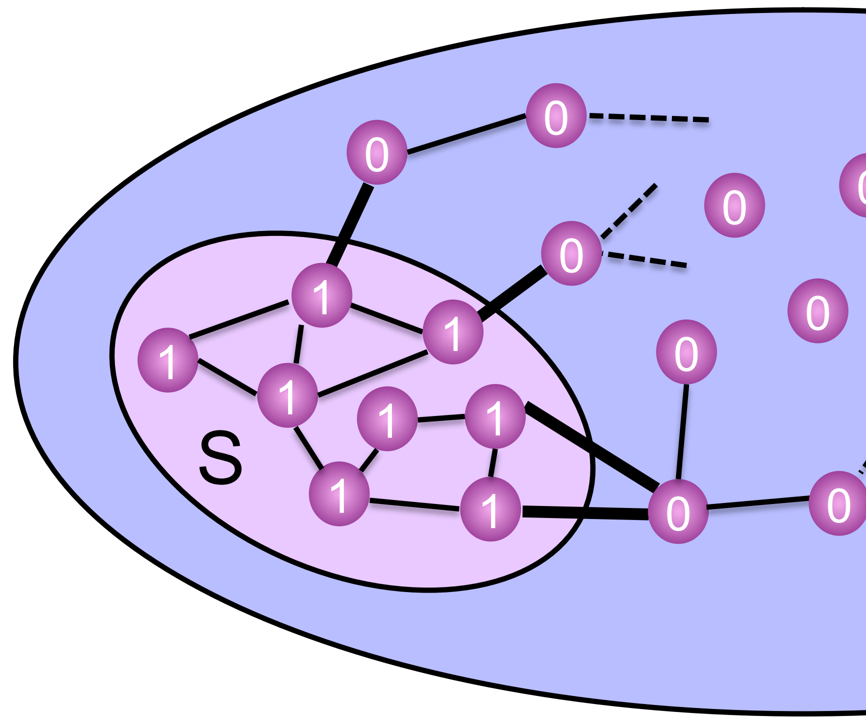
$$x^T L x = \sum_{(a,b)\in E} (x(a) - x(b))^2 = |\text{boundary}(S)|$$

Cluster Quality

$$\frac{\text{Number of edges leaving S}}{\text{Size of S}}$$

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

$$\stackrel{\text{def}}{=} \Phi(S)$$ (sparsity)



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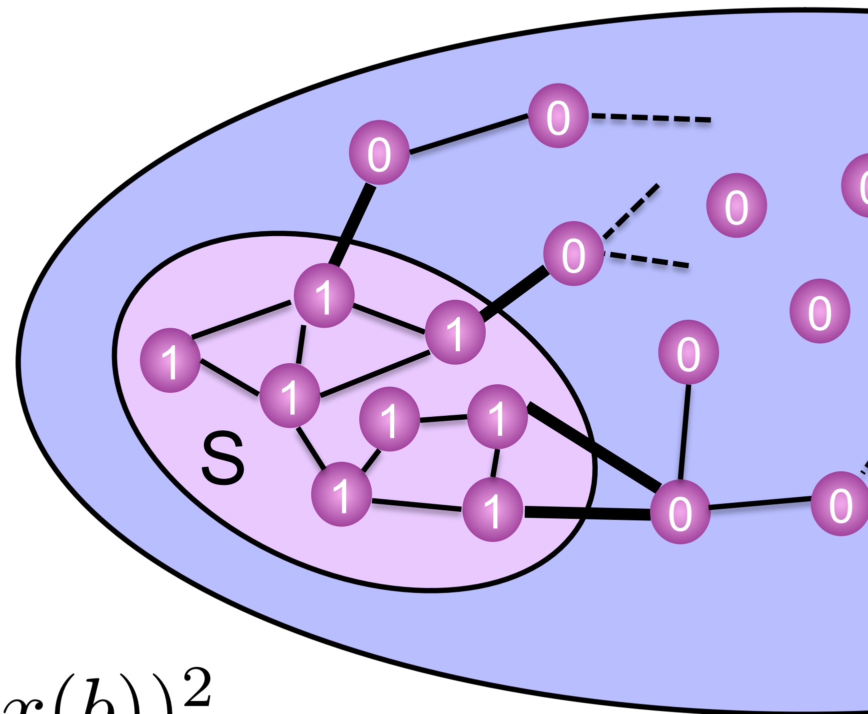
$$= \frac{x^T L x}{x^T x} = \frac{\sum_{(a,b)\in E} (x(a) - x(b))^2}{\sum_a x(a)^2}$$



The Rayleigh Quotient of x with respect to L

Spectral Graph Theory

A n-by-n symmetric matrix has n real eigenvalues $\lambda_1 \leq \lambda_2 \cdots \leq \lambda_n$ and eigenvectors $v_1, ..., v_n$ such that

$$Lv_i = \lambda_i v_i$$

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These eigenvalues and eigenvectors tell us a lot about a graph!

Theorems
Algorithms
Heuristics

The Rayleigh Quotient and Eigenvalues

A n-by-n symmetric matrix has n real eigenvalues $\lambda_1 \leq \lambda_2 \cdots \leq \lambda_n$ and eigenvectors $v_1, ..., v_n$ such that

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Courant-Fischer Theorem:

$$\lambda_1 = \min_{x \neq 0} \frac{x^T L x}{x^T x} \qquad v_1 = \arg\min_{x \neq 0} \frac{x^T L x}{x^T x}$$

The Courant Fischer Theorem

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$$\lambda_2 = \min_{x \perp v_1} \frac{x^T L x}{x^T x} \qquad v_2 = \arg\min_{x \perp v_1} \frac{x^T L x}{x^T x}$$

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$$\boxed{\begin{aligned} \lambda_k &= \min_{x \perp v_1, \ldots, v_{k-1}} \frac{x^T L x}{x^T x} \\ v_k &= \arg\min_{x \perp v_1, \ldots, v_{k-1}} \frac{x^T L x}{x^T x} \end{aligned}}$$

The first eigenvalue

$$\lambda_1 = \min_{x \neq 0} \frac{x^T L x}{x^T x}$$

$$= \min_{x \neq 0} \frac{\sum_{(a,b) \in E} (x(a) - x(b))^2}{\|x\|^2}$$

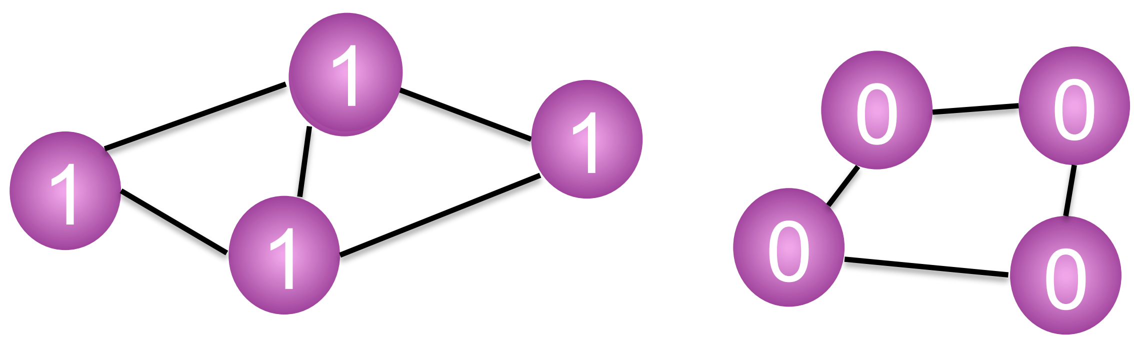
Setting $x(a) = 1$ for all a

We find $\lambda_1 = 0$ and $v_1 = \mathbf{1}$

The second eigenvalue

$\lambda_2 > 0$ if and only if G is connected

Proof: if G is not connected,
are two functions with Rayleigh quotient zero



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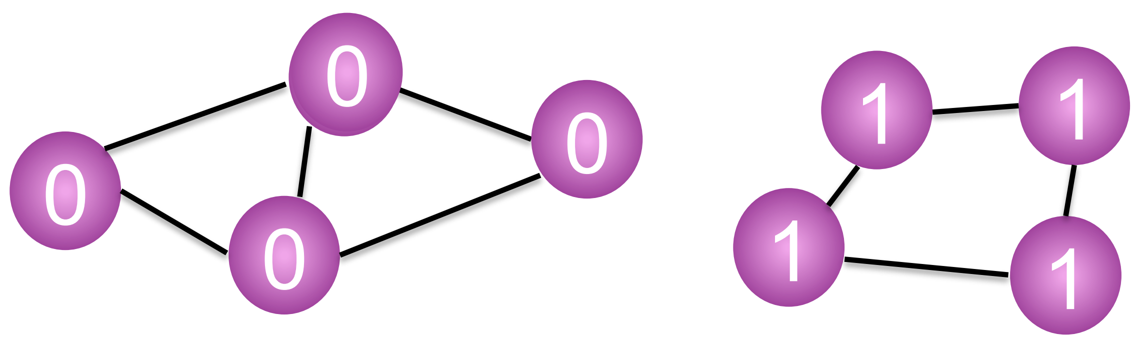

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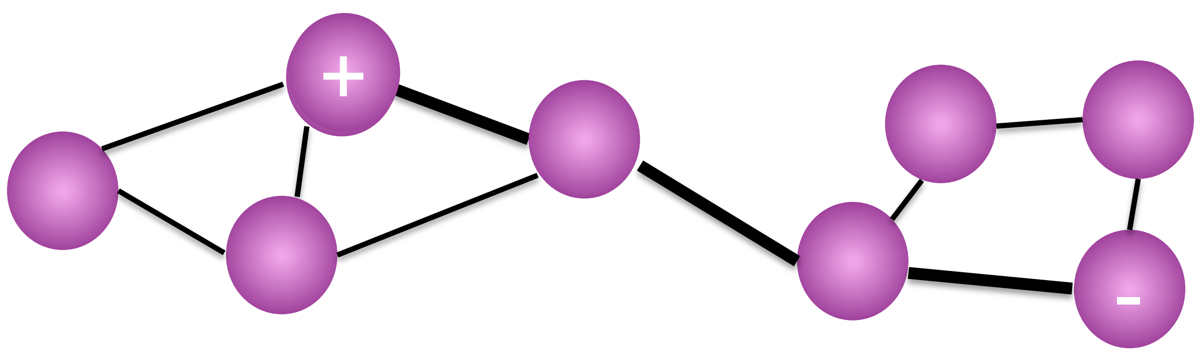
Proof: if G is connected,

$x \perp \mathbf{1}$ means $\sum_a x(a) = 0$

So must be an edge (a,b) for which

$x(a) < x(b)$ and so $(x(a) - x(b))^2 > 0$



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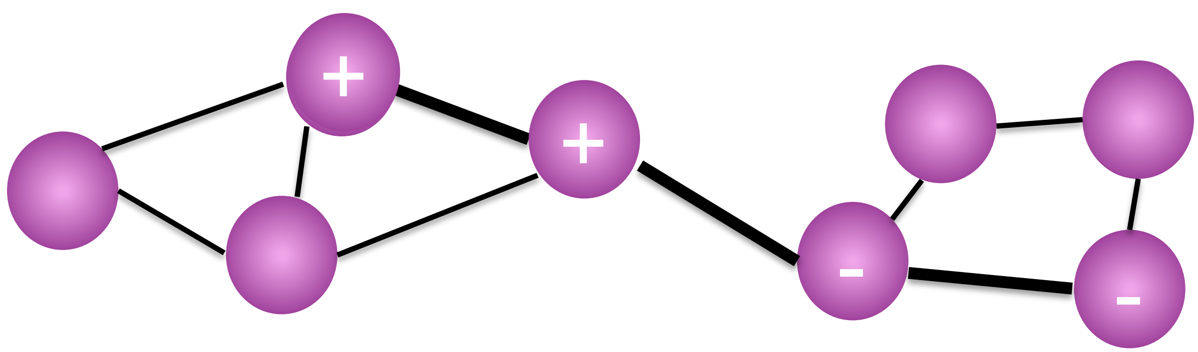

The second eigenvalue

$\lambda_2 > 0$ if and only if G is connected

Fiedler ('73) called λ_2
"the algebraic connectivity of a graph"
The further from 0, the more connected.

Cheeger's Inequality [Cheeger '70]

[Alon-Milman '85, Jerrum-Sinclair '89, Diaconis-Stroock '91]

1. λ_2 is big if and only if G does not have good clusters.

2. If λ_2 is small, can use v_2 to find a good cluster.

Cheeger's Inequality [Cheeger '70]

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1. λ_2 is big if and only if G does not have good clusters.

When every vertex has d edges,

$$\lambda_2/2 \leq \min_{|S| \leq n/2} \Phi(S) \leq \sqrt{2d\lambda_2}$$

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

Cheeger's Inequality [Cheeger '70]

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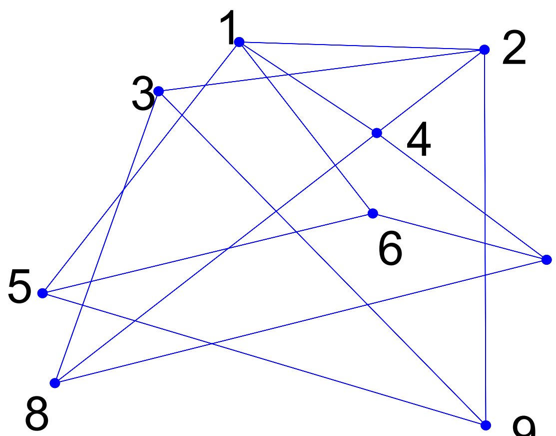
In a moment…

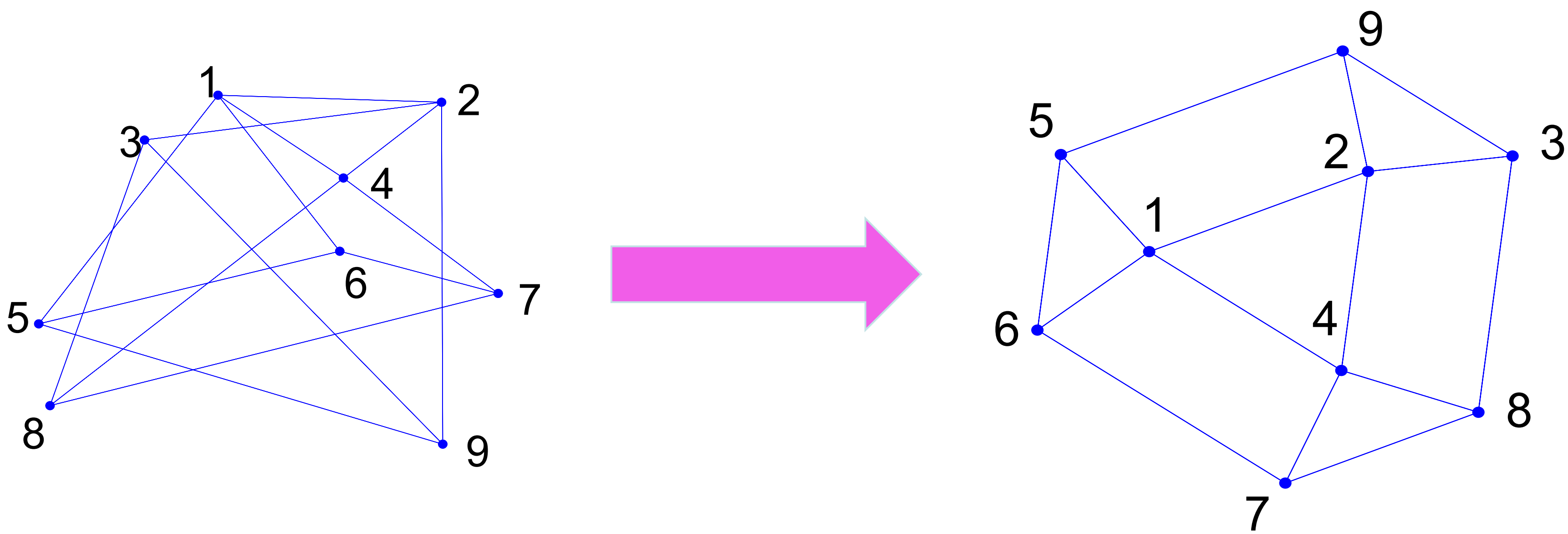
Spectral Graph Drawing [Hall '70]



Arbitrary
Drawing

Spectral Graph Drawing [Hall '70]

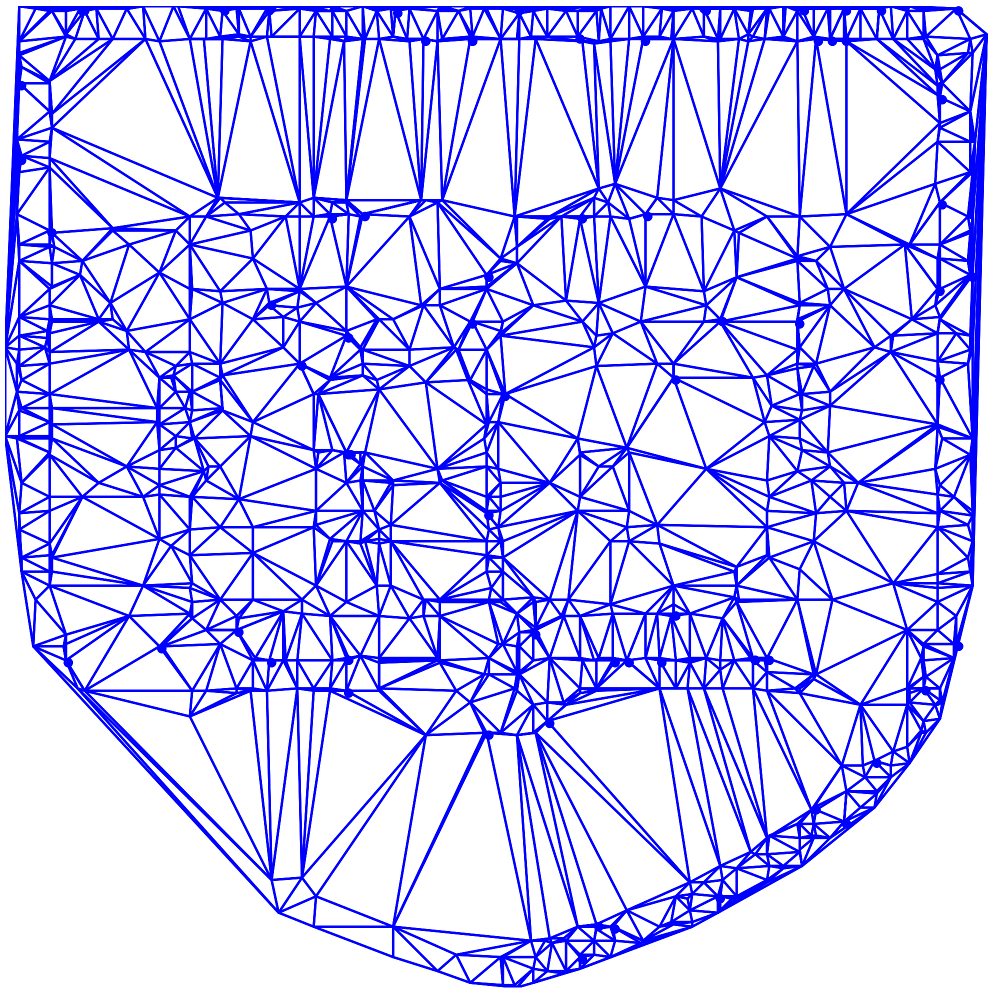
Plot vertex a at $(v_2(a), v_3(a))$
draw edges as straight lines



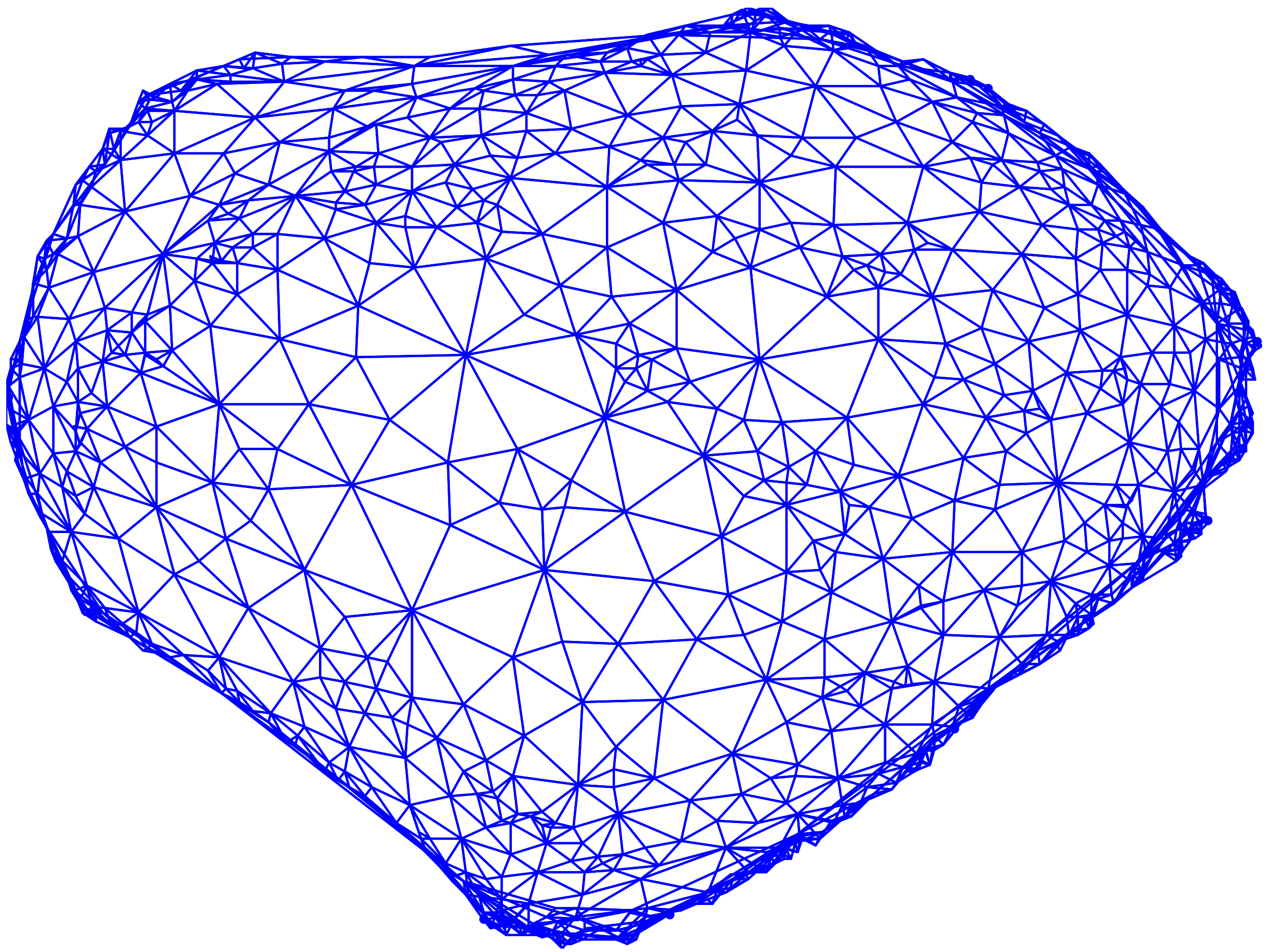
Arbitrary Drawing

Spectral Drawing

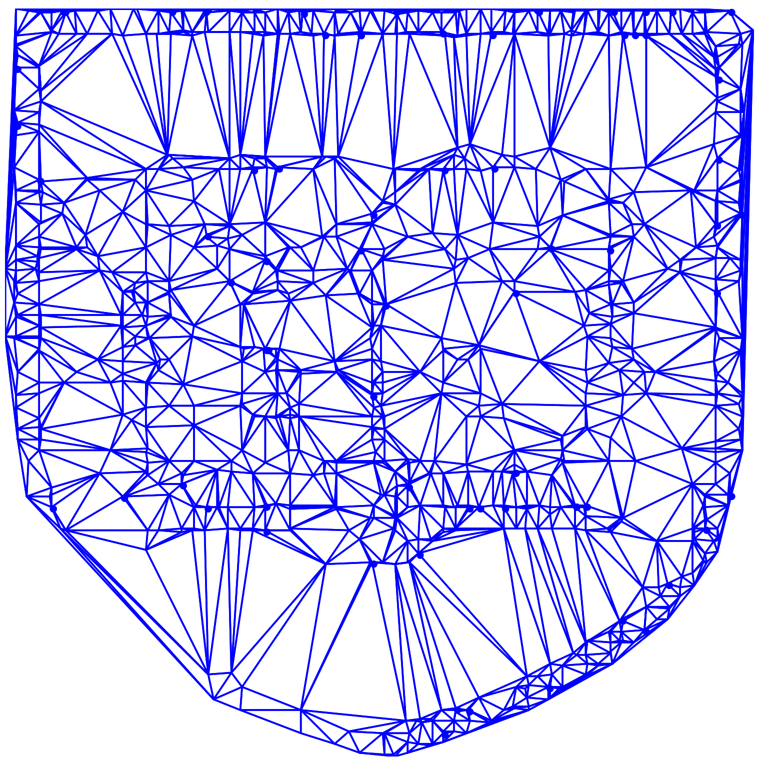
A Graph

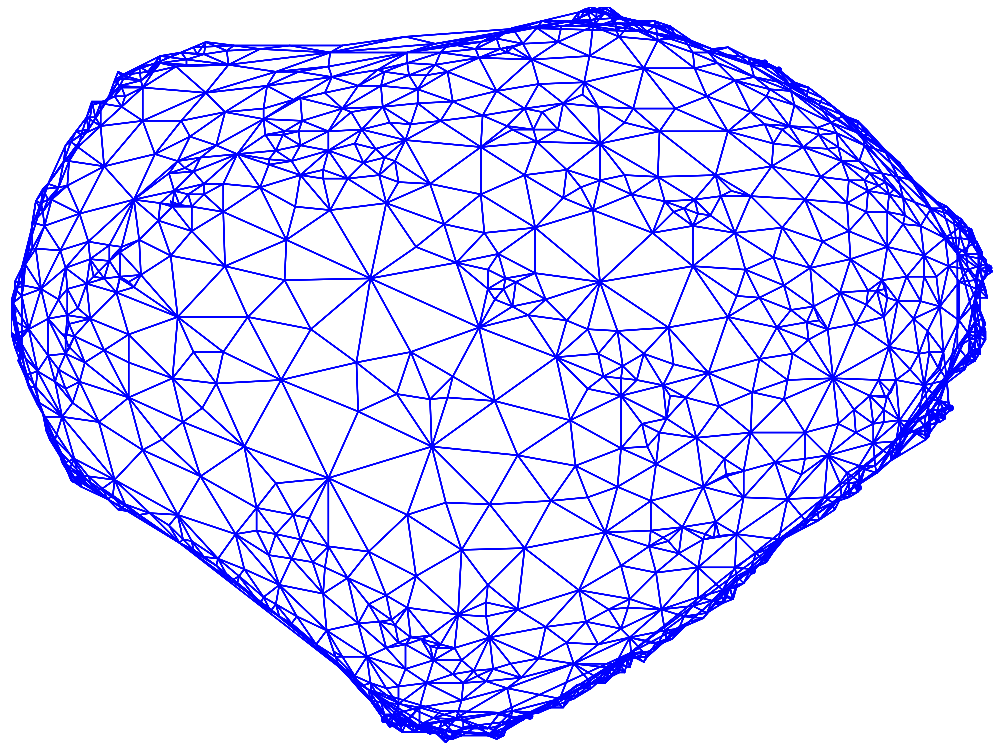


Drawing of the graph using v_2, v_3

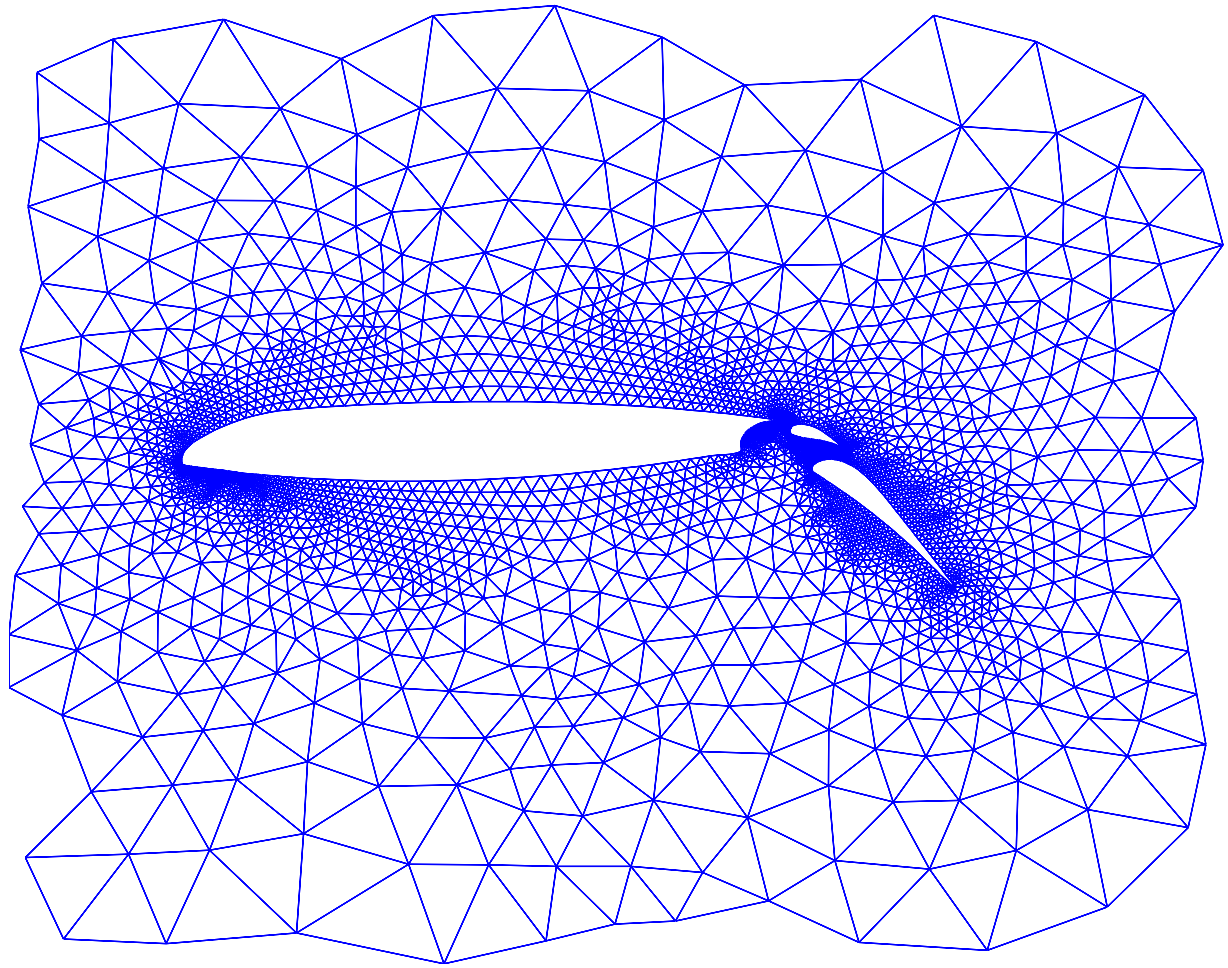


Plot vertex a at $(v_2(a), v_3(a))$

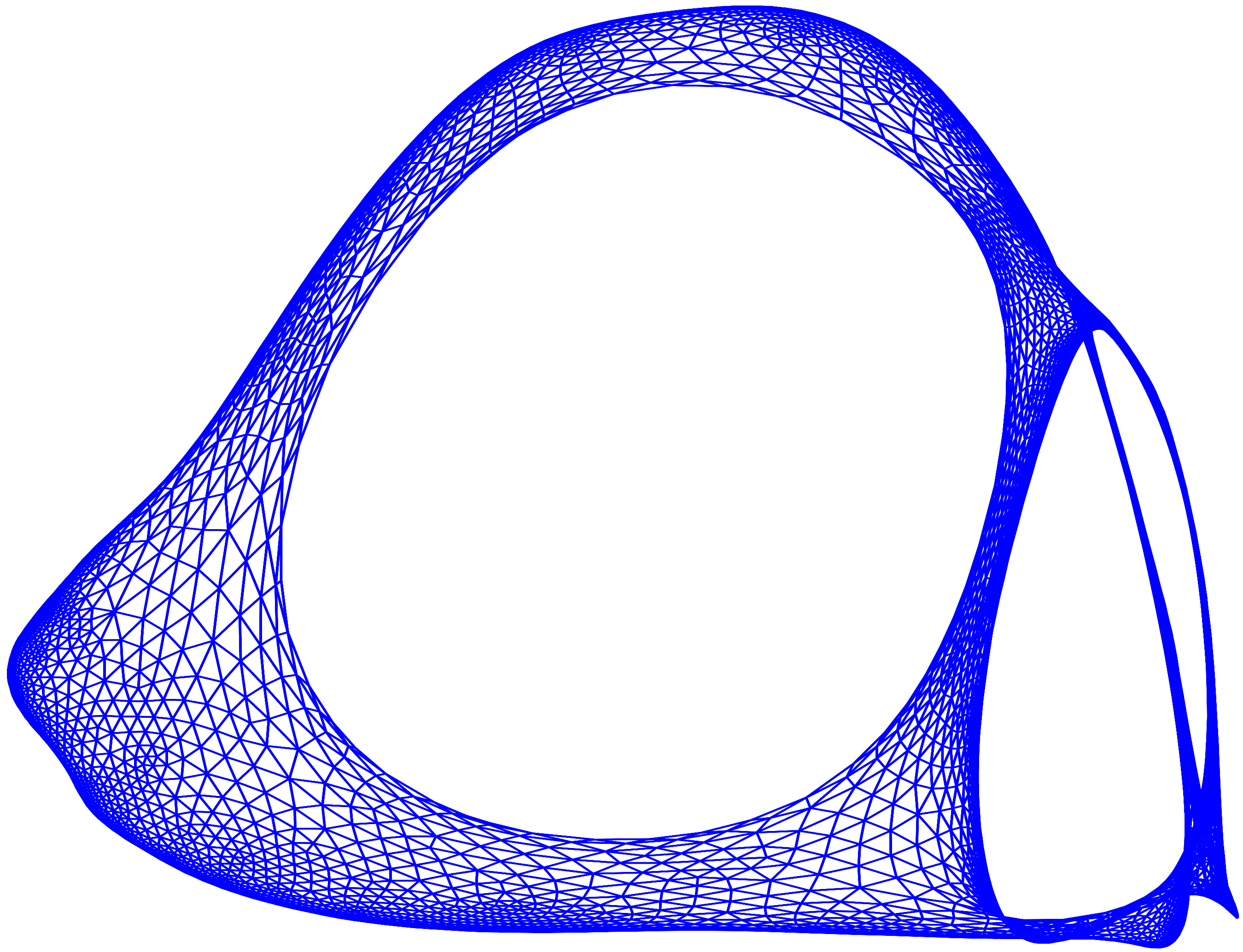




The Airfoil Graph, original coordinates



The Airfoil Graph, spectral coordinates



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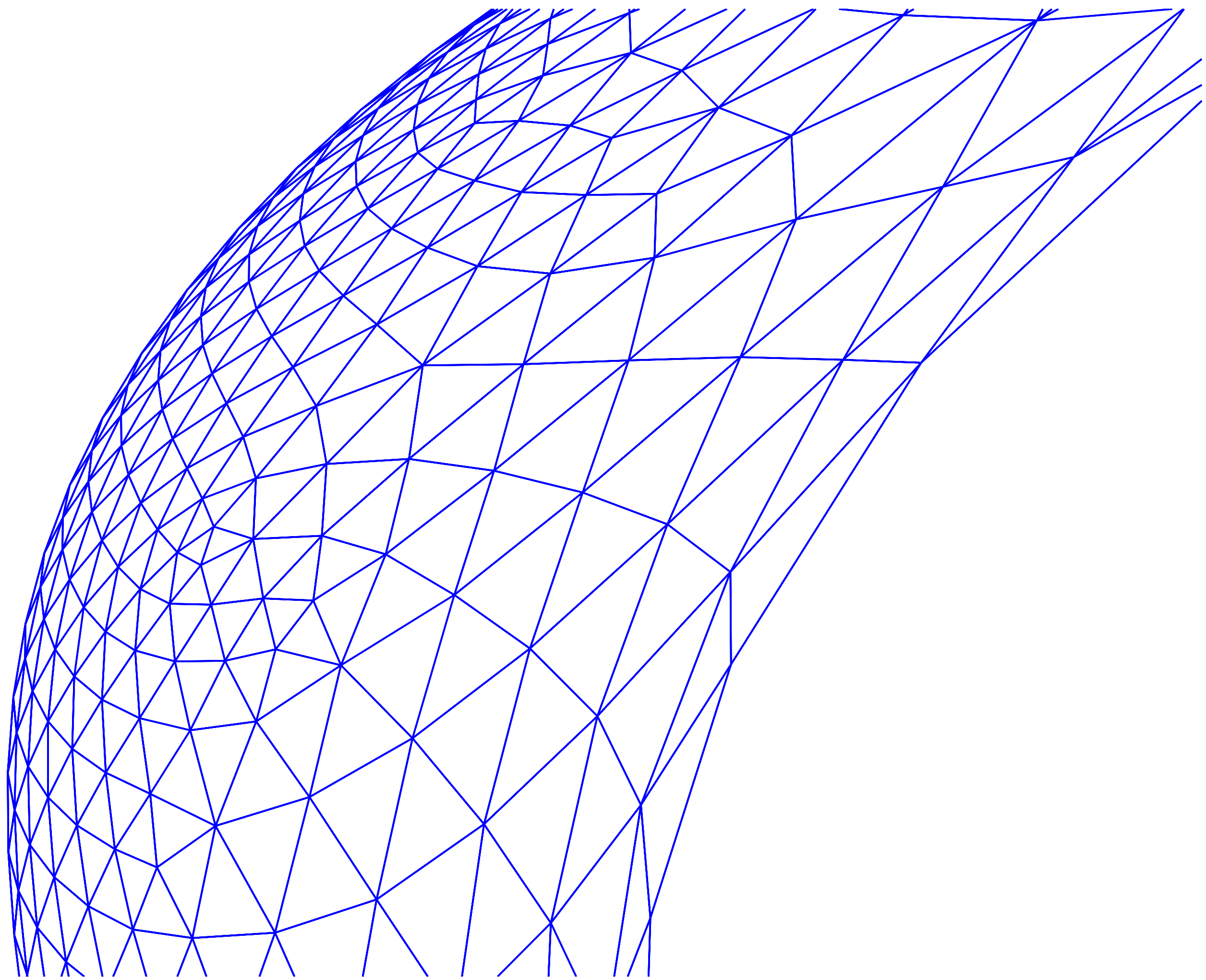
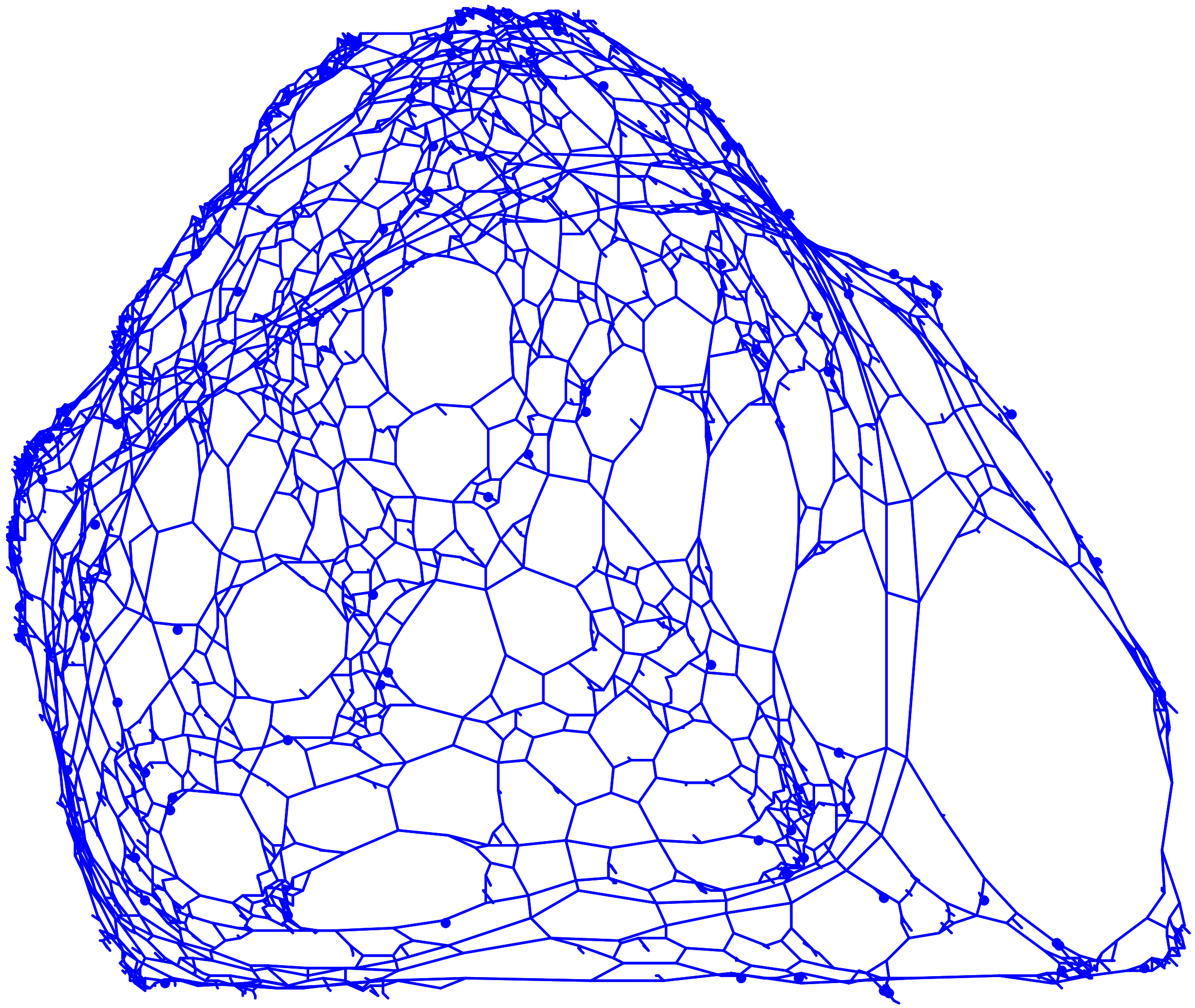
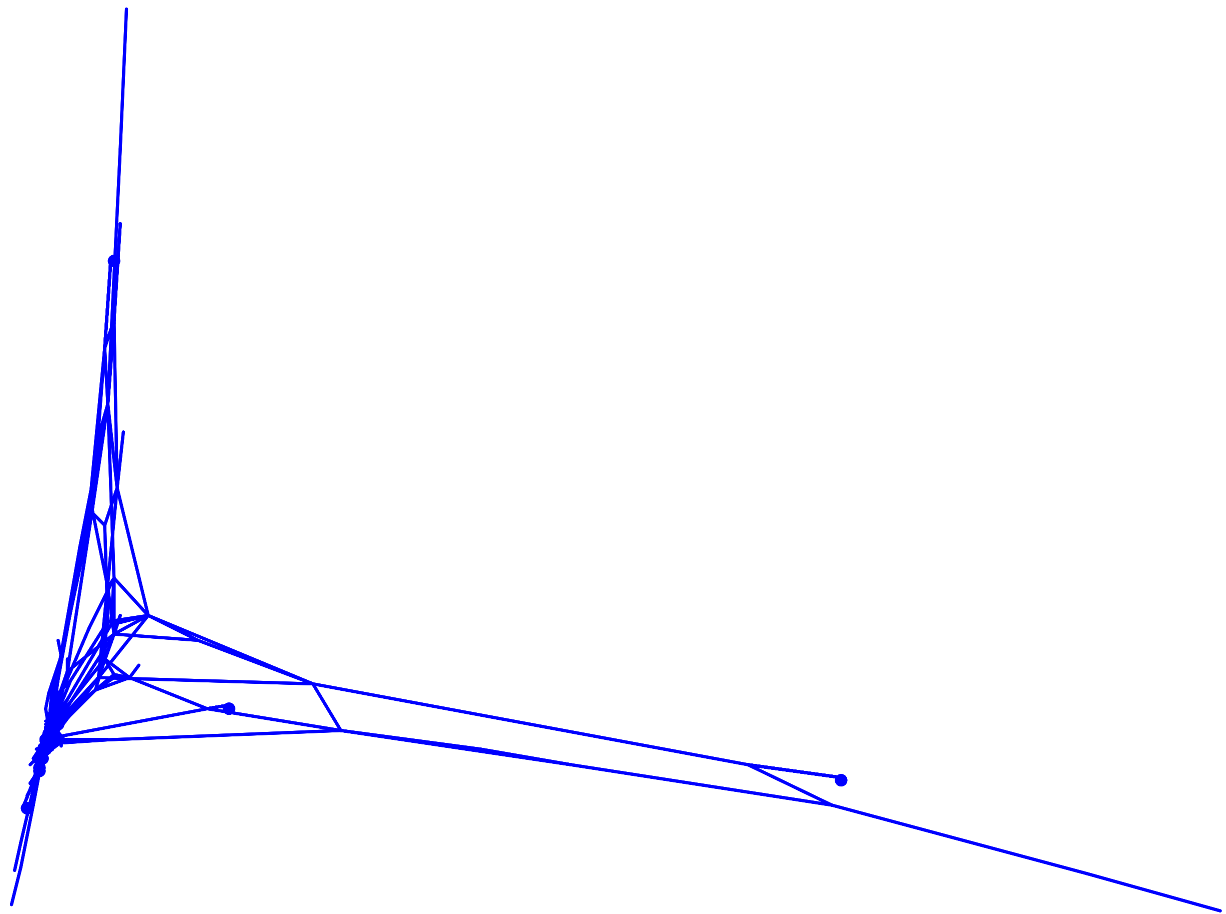


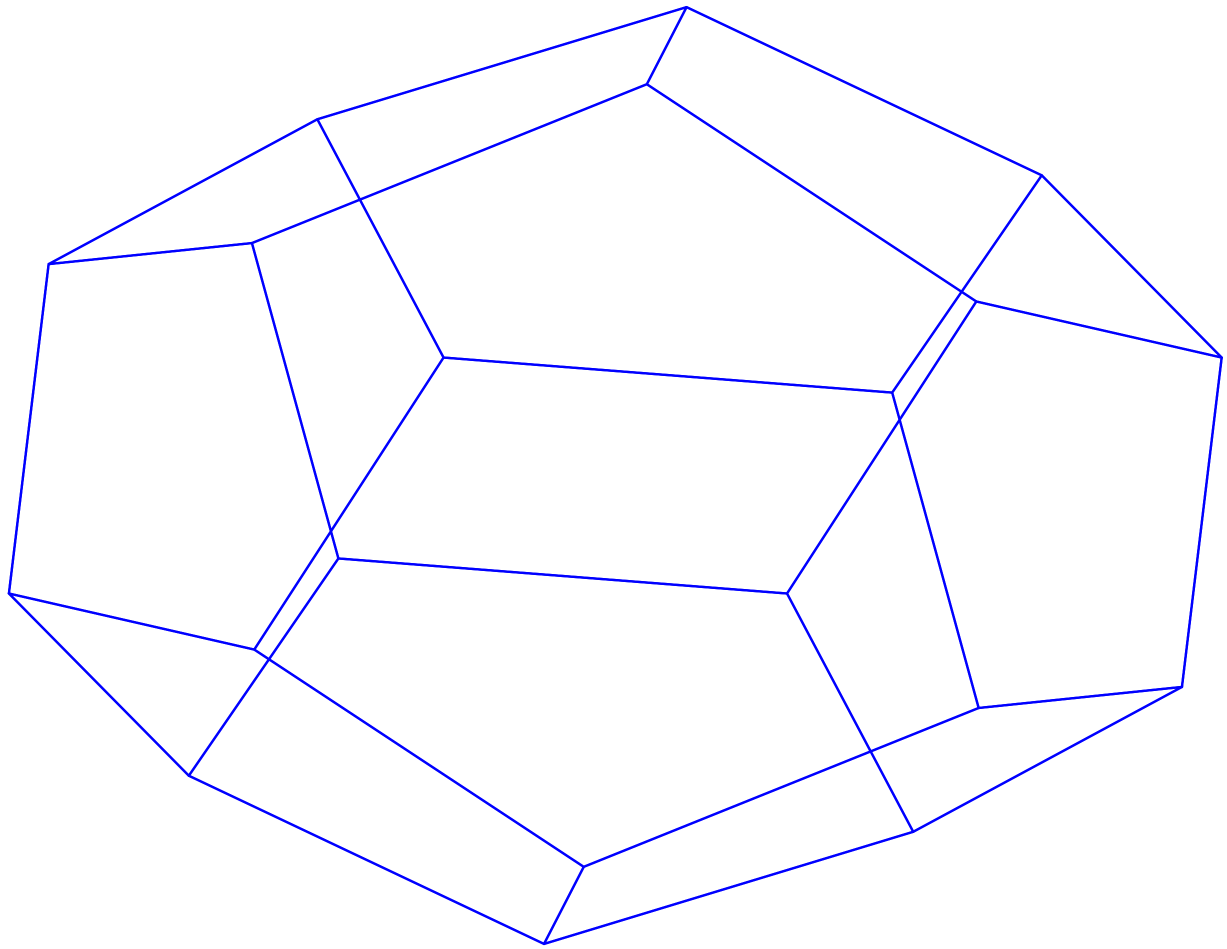
Spectral drawing of Streets in Rome



Spectral drawing of Erdos graph: edge between co-authors of papers



Dodecahedron



Best embedded by first three eigenvectors

Spectral graph drawing: Tutte justification

Condition for eigenvector $Lx = \lambda x$

Gives $\vec{x}(a) = \frac{1}{d_a - \lambda} \sum_{(a,b) \in E} \vec{x}(b)$ for all a

λ small says $\vec{x}(a)$ near average of neighbors

Spectral graph drawing: Tutte justification

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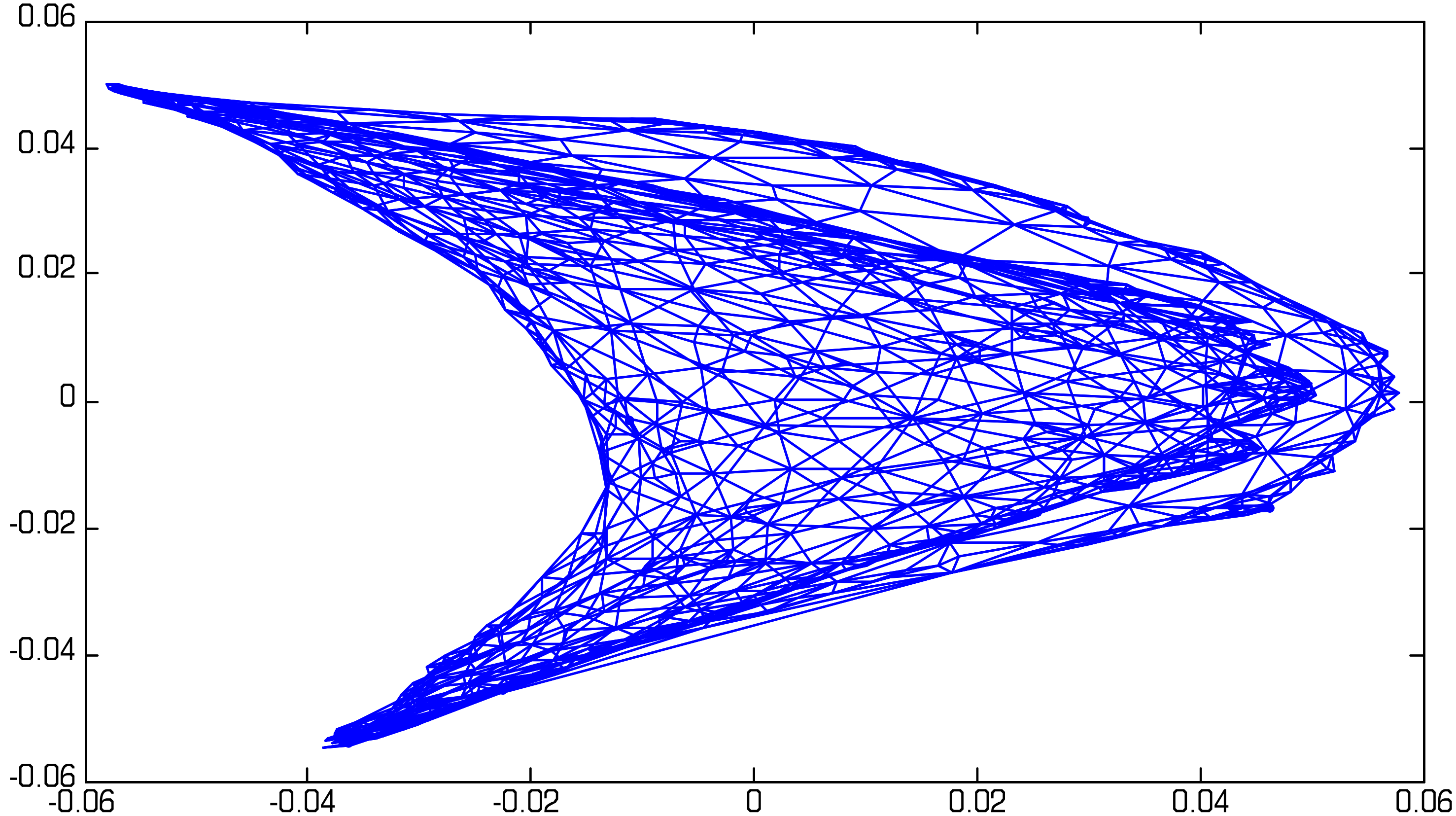
λ small says $\vec{x}(a)$ near average of neighbors

For planar graphs:

$\lambda_2 \leq 8d/n$ [S-Teng '96]

$\lambda_3 \leq O(d/n)$ [Kelner-Lee-Price-Teng '09]

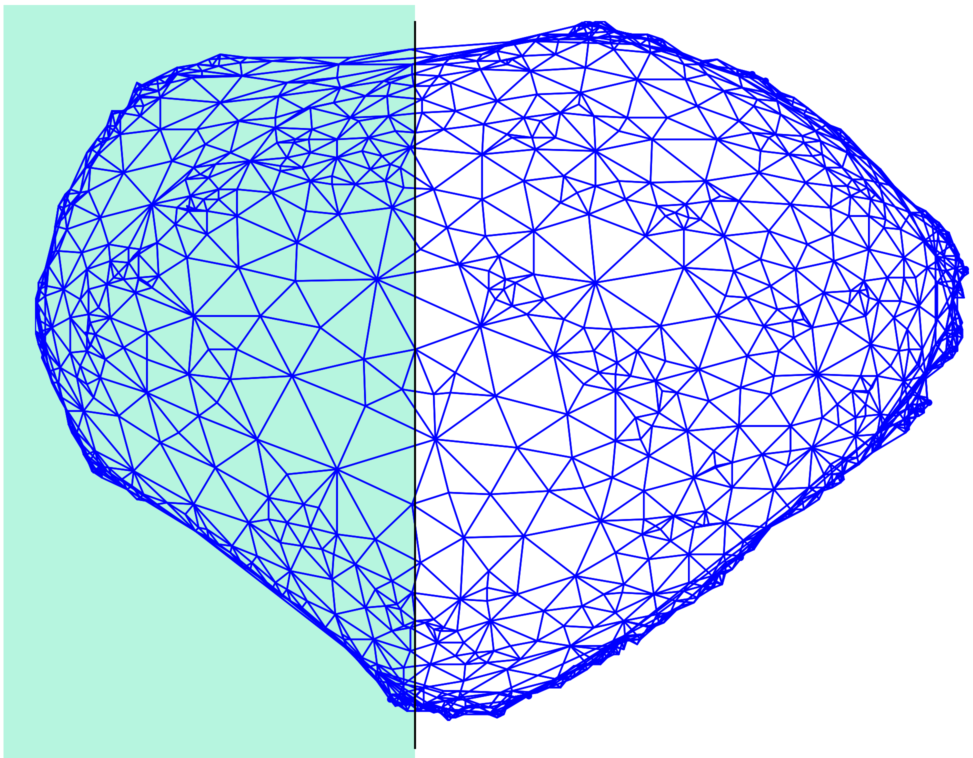
Small eigenvalues are not enough



Plot vertex a at $(v_3(a), v_4(a))$

Spectral Graph Partitioning

[Donath-Hoffman ‘72, Barnes ‘82, Hagen-Kahng ‘92]



$S = \{a : v_2(a) \leq t\}$ for some t

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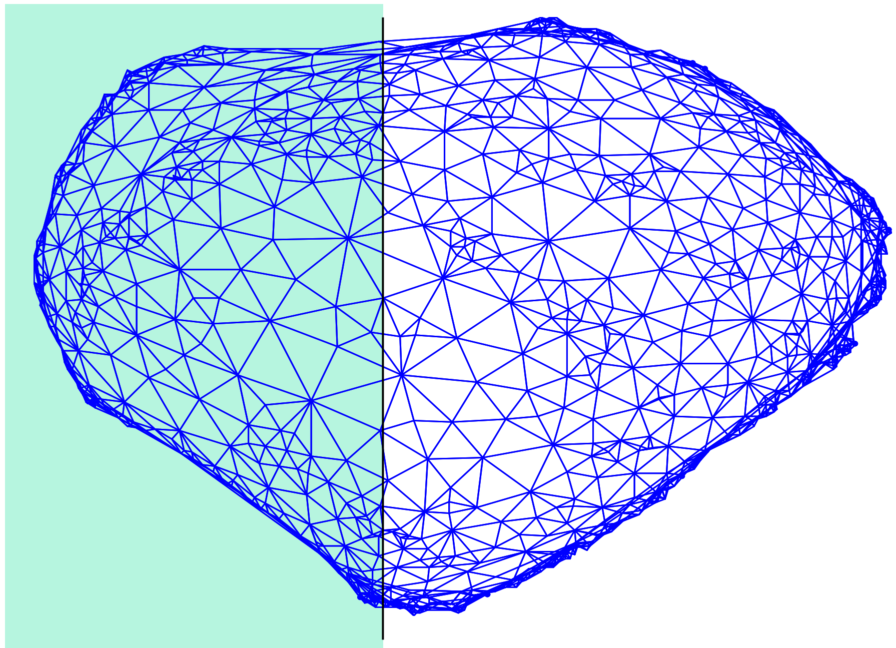


$S = \{a : v_2(a) \leq t\}$ for some t

Cheeger's Inequality says there is a t so that

$$\Phi(S) \leq \sqrt{2d\lambda_2}$$

Major topics in spectral graph theory

Graph Isomorphism:
determining if two graphs are the same

Independent sets:
large sets of vertices containing no edges

Graph Coloring:
so that edges connect different colors

Major topics in spectral graph theory

- Graph Isomorphism
- Independent sets
- Graph Coloring
- Behavior under graph transformations
- Random Walks and Diffusion
- PageRank and Hits
- Colin de Verdière invariant
- Special Graphs
  - from groups
  - from meshes
- Machine learning
- Image processing

Solving linear equations in Laplacians

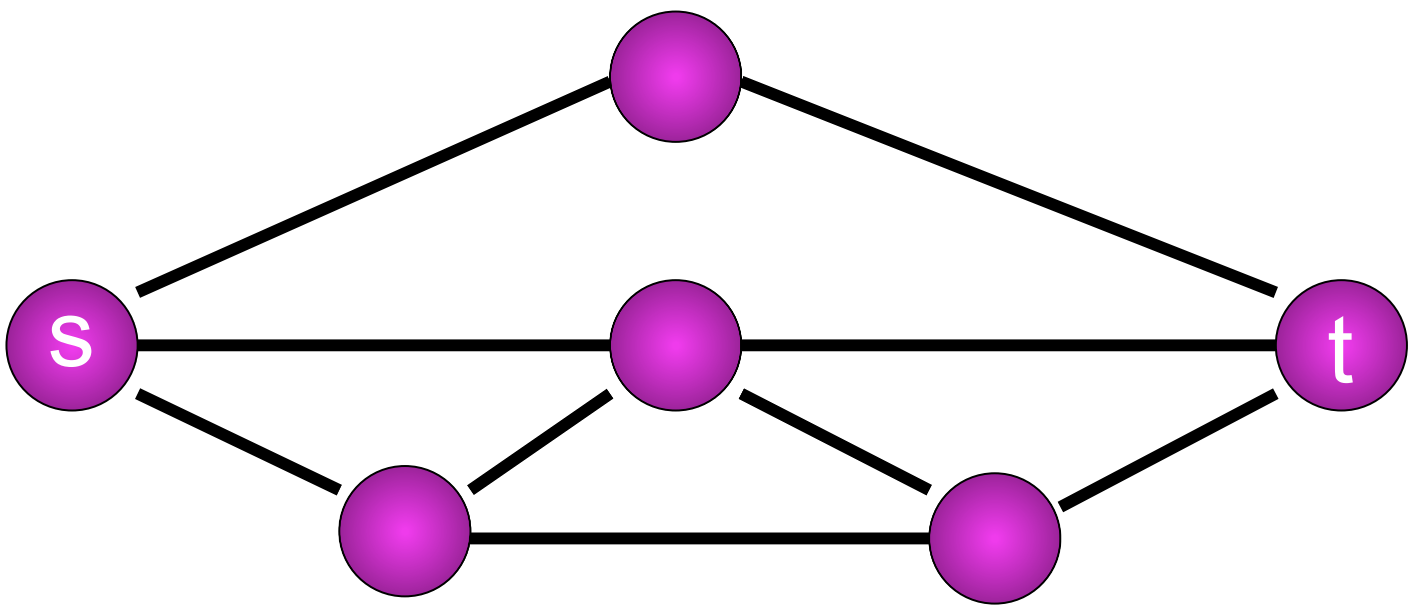
For energy minimization and computation of eigenvectors and eigenvalues

Can do it in time nearly-linear in the number of edges in the graph!

A powerful computational primitive.

Maximum flow problem

Send as much stuff as possible from s to t.
At most one unit can go through each edge.



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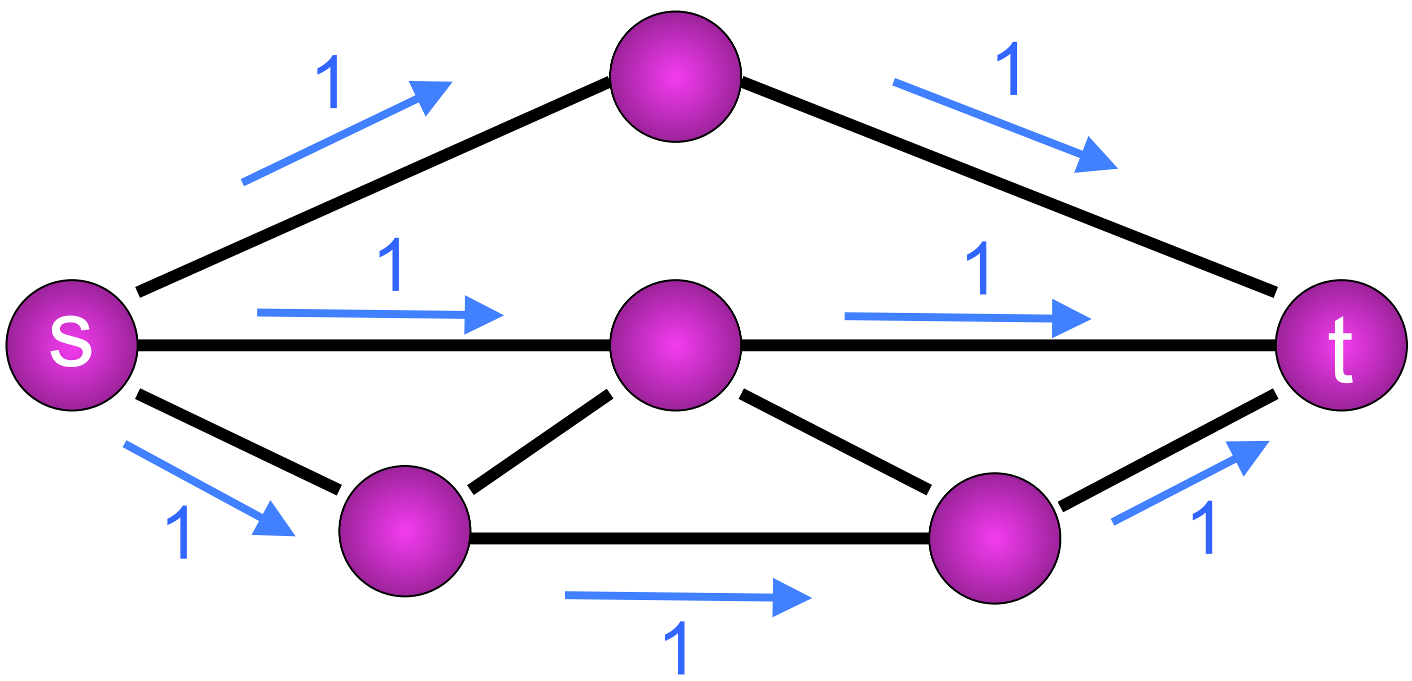

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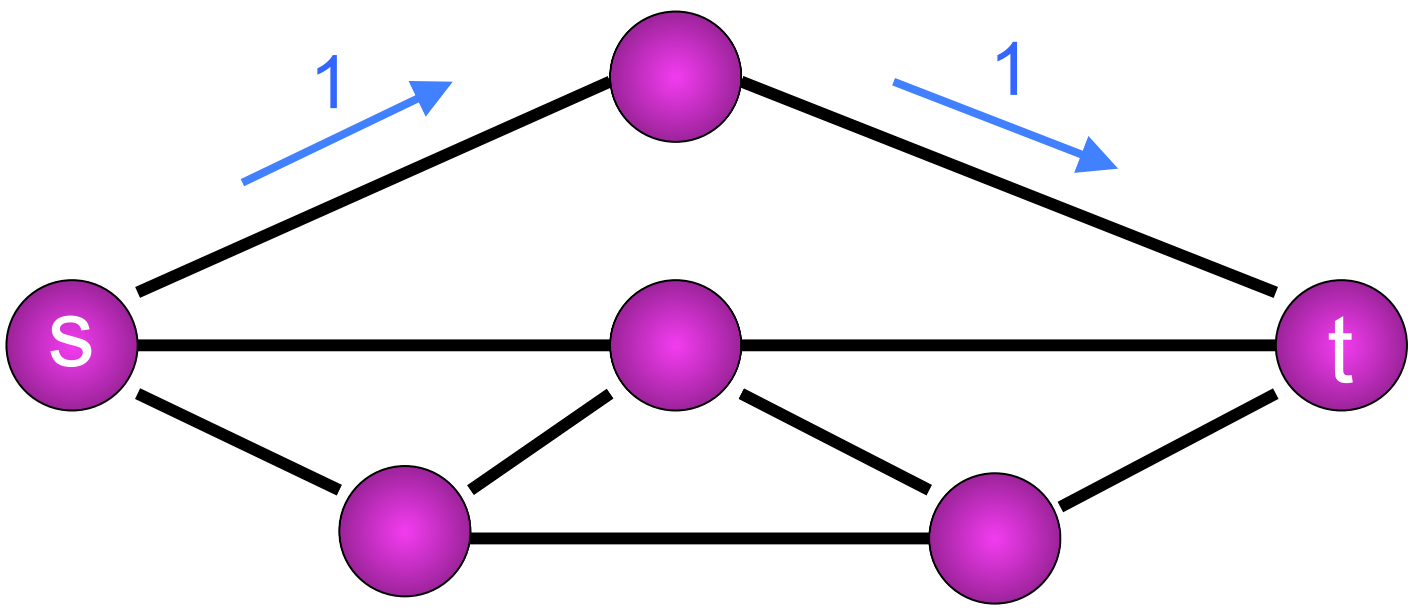

Standard approach: incrementally add flow paths

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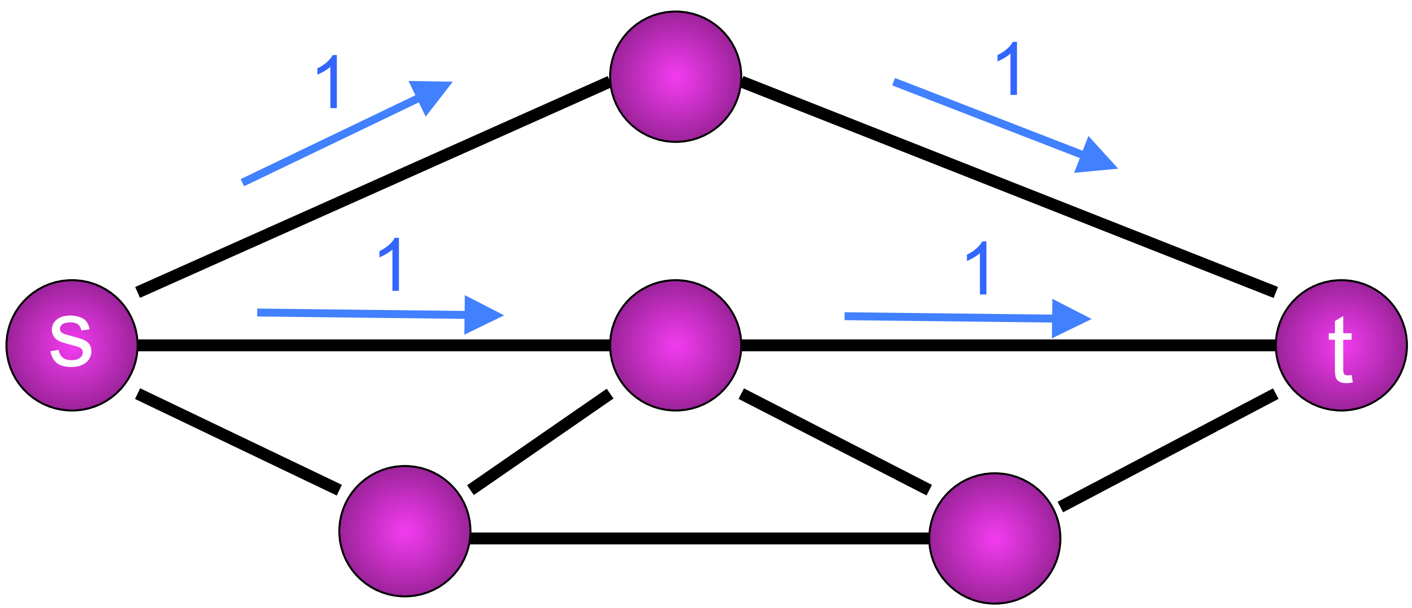

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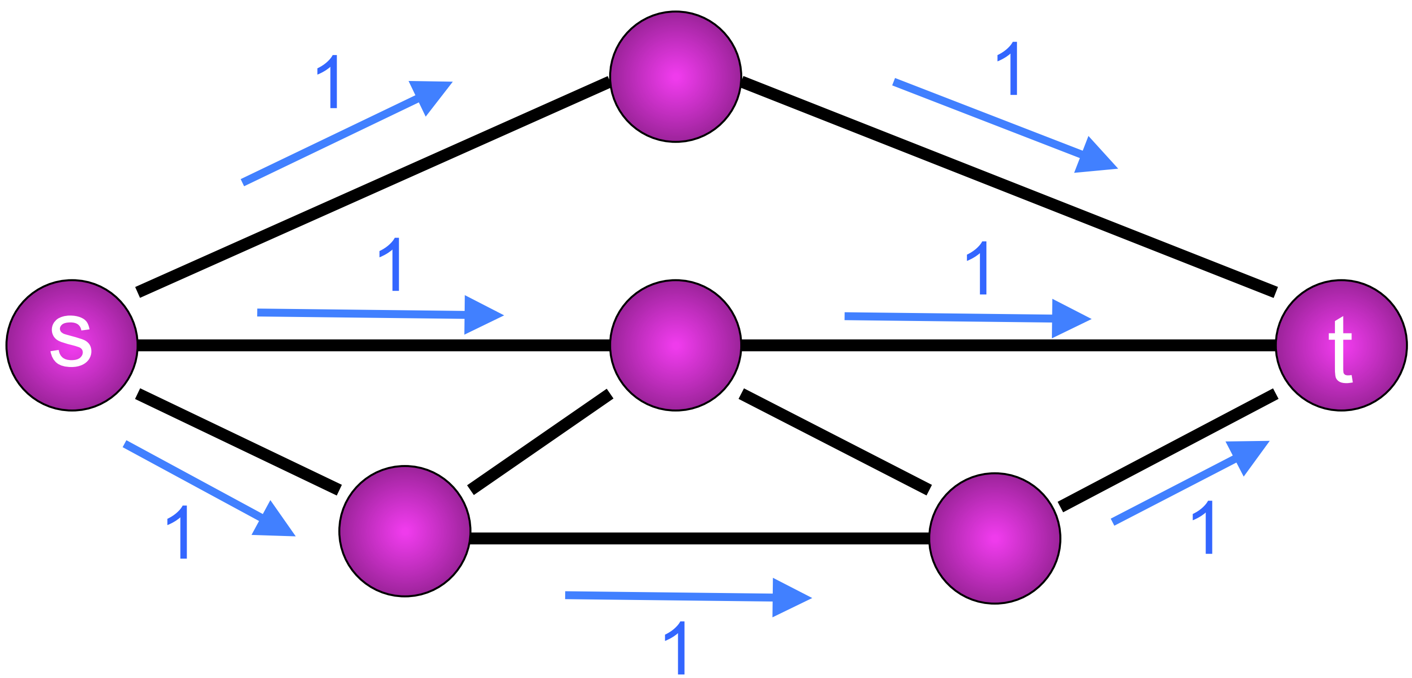

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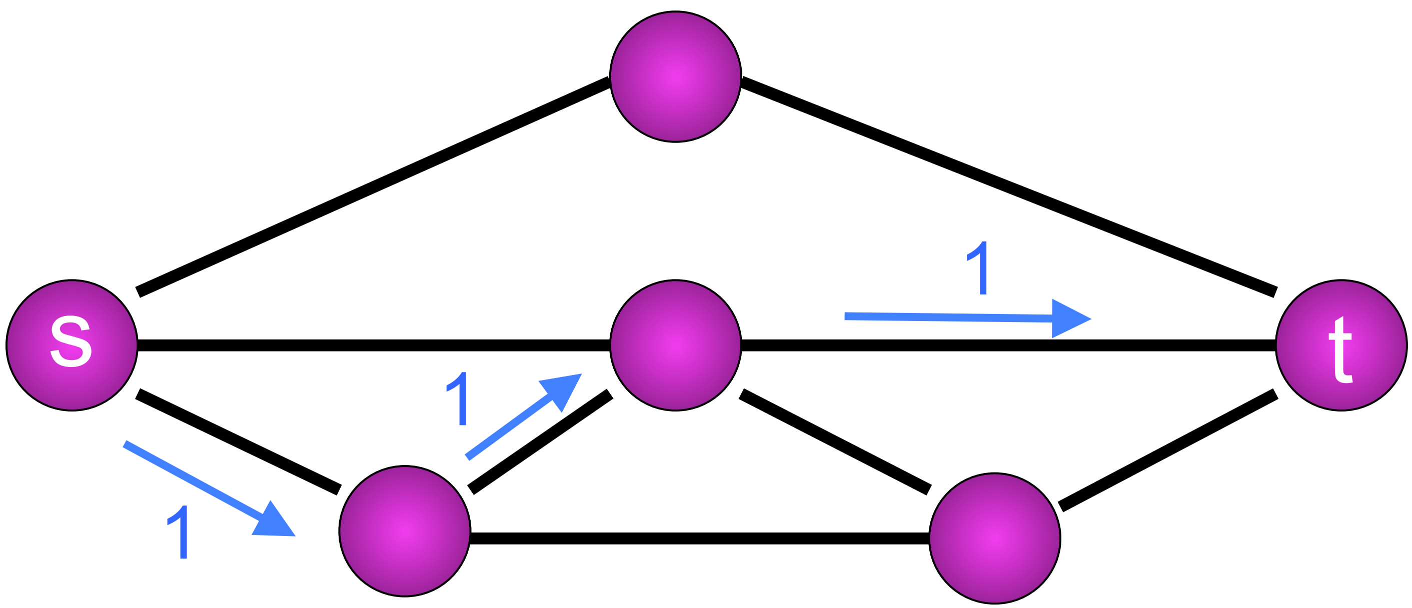
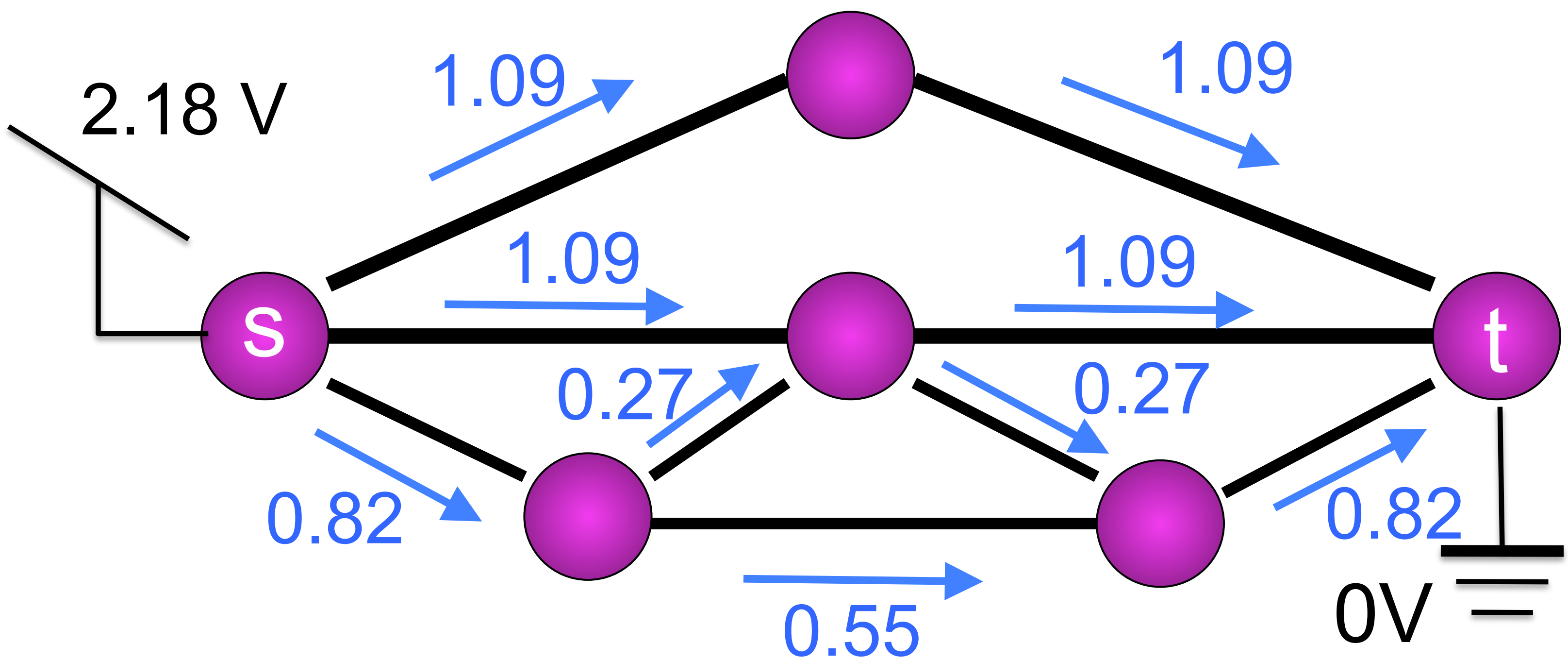


Standard approach: incrementally add flow paths
Issue: sometimes requires backtracking

Maximum flow problem, electrical approach

[Christiano-Kelner-Madry-S-Teng '11]

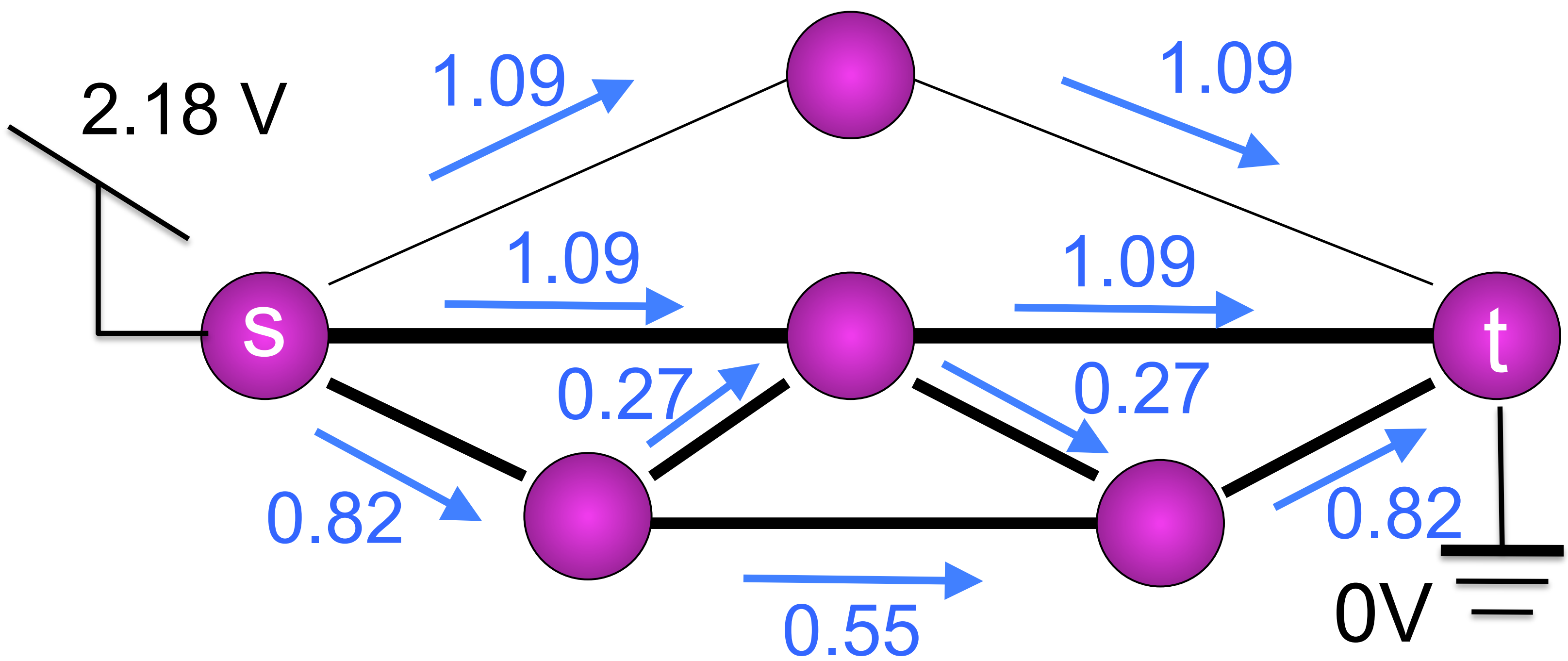
1. Try the electrical flow.



Maximum flow problem, electrical approach

[Christiano-Kelner-Madry-S-Teng '11]

1. Try the electrical flow.
2. Increase resistance when too much flow



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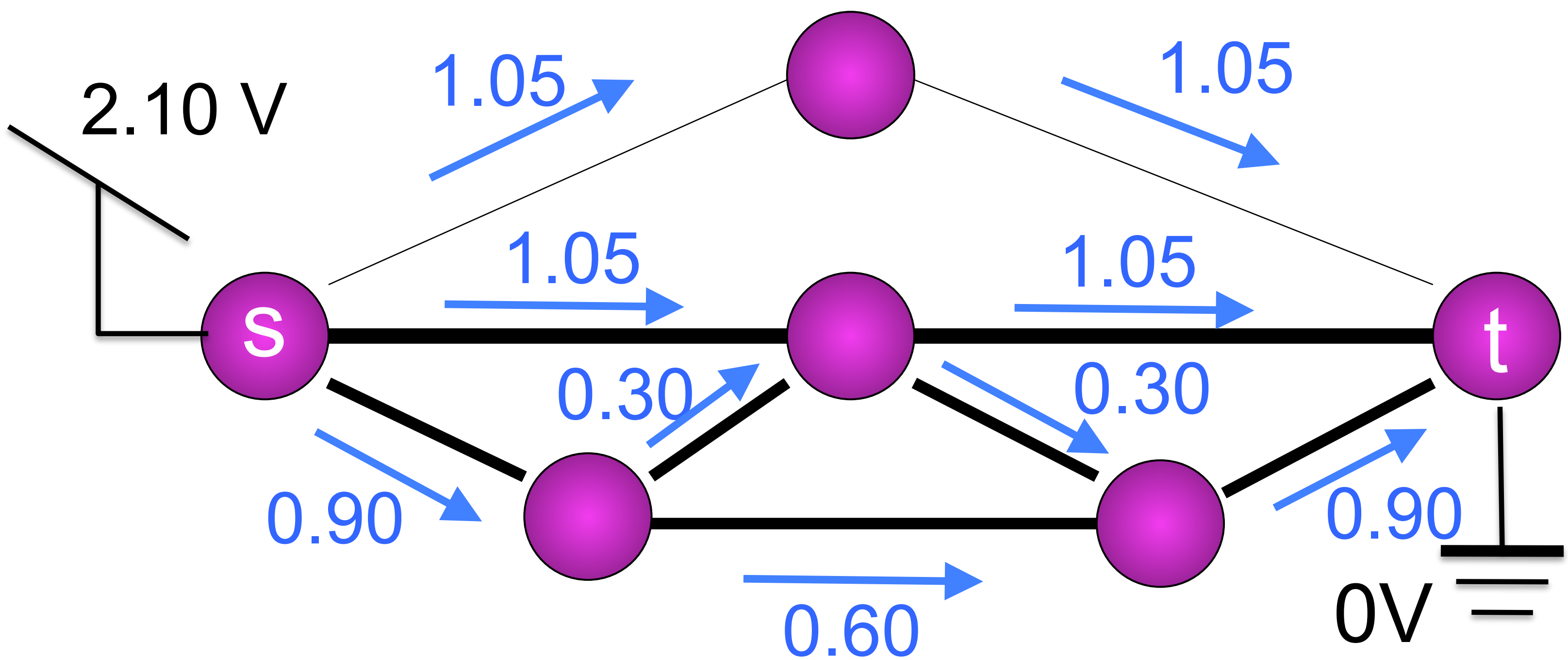

Solving linear equations in Laplacians

For energy minimization and
computation of eigenvectors and eigenvalues

Can do it in time nearly-linear in the
number of edges in the graph!

Key ideas:
- how to approximate a graph by a tree
  - or by a very sparse graph
- random matrix theory
- numerical linear algebra

Approximating Graphs

A graph H is an ϵ-approximation of G if

for all x

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

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To solve linear equations quickly,
approximate G by a simpler graph H

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A very strong notion of approximation
Preserves all electrical and spectral properties

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Theorem [Batson-S-Srivastava '09]

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

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A powerful technique in linear algebra

many applications

To learn more

Lectures 2 and 3:

- More precision
- More notation
- Similar sophistication

To learn more

See my lecture notes from
"Spectral Graph Theory"
and
"Graphs and Networks"