Laplacian Matrices of Graphs: Spectral and Electrical Theory

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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
Examples of Graphs
Examples of Graphs
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
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
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
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

When stretched to length $\ell$
potential energy is $\ell^2 / 2$
Graphs as Spring Networks

Nail down some vertices, let rest settle.

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

\[ x(a) \]

Energy minimized when free vertices are averages of neighbors

\[ \overrightarrow{x}(a) = \frac{1}{d_a} \sum_{(a,b) \in E} \overrightarrow{x}(b) \]

\( d_a \) 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
Tutte’s Theorem ‘63

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3-connected:
cannot break graph by cutting 2 edges
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

View edges as resistors connecting vertices.

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

Current flow measures strength of connection between endpoints.

More short disjoint paths lead to higher flow.
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

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
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
The Laplacian quadratic form

\[ \sum_{(a,b) \in E} (x(a) - x(b))^2 \]
The Laplacian matrix of a graph

\[ x^T L x = \sum_{(a,b) \in E} (x(a) - x(b))^2 \]
The Laplacian matrix of a graph

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

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

Solve equation of form

\[ L x = b \]
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

\[
x^T L x = \sum_{(a,b) \in E} w_{a,b} (x(a) - x(b))^2
\]
Weighted Graphs

Edge \((a, b)\) assigned a non-negative real weight
\(w_{a,b} \in \mathbb{R}\) measuring
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\[
x^T L x = \sum_{(a,b) \in E} w_{a,b} (x(a) - x(b))^2
\]

*I’ll show the matrix entries tomorrow*
Measuring boundaries of sets

Boundary: edges leaving a set
Measuring boundaries of sets

Boundary: edges leaving a set
Measuring boundaries of sets

Boundary: edges leaving a set

Characteristic Vector of $S$:

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

Boundary: edges leaving a set

Characteristic Vector of S:

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

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

Number of edges leaving $S$
\[
\frac{\text{Size of } S}{\left| \text{boundary}(S) \right|}
\]
\[
= \frac{\left| \text{boundary}(S) \right|}{|S|}
\]
\[
\text{def } \Phi(S) \quad \text{(sparsity)}
\]
Cluster Quality

Number of edges leaving \( S \) \over \text{Size of } S

\[
= \frac{|\text{boundary}(S)|}{|S|}
\]

def \[ \Phi(S) \] \text{ (sparsity)}

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

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 $v_1, \ldots, v_n$ such that

$$Lv_i = \lambda_i v_i$$
Spectral Graph Theory

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

$$Lv_i = \lambda_i v_i$$

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 $v_1, \ldots, v_n$ such that

$$Lv_i = \lambda_i v_i$$

Courant-Fischer Theorem:

$$\lambda_1 = \min_{x \neq 0} \frac{x^T L x}{x^T x} \quad \quad v_1 = \arg \min_{x \neq 0} \frac{x^T L x}{x^T x}$$
The Courant Fischer Theorem

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

\[ \lambda_2 = \min_{x \perp v_1} \frac{x^T L x}{x^T x} \]

\[ v_1 = \arg \min_{x \neq 0} \frac{x^T L x}{x^T x} \]

\[ v_2 = \arg \min_{x \perp v_1} \frac{x^T L x}{x^T x} \]
The Courant Fischer Theorem

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

\[ v_1 = \arg \min_{x \neq 0} \frac{x^T L x}{x^T x} \]

\[ \lambda_2 = \min_{x \perp v_1} \frac{x^T L x}{x^T x} \]

\[ v_2 = \arg \min_{x \perp v_1} \frac{x^T L x}{x^T x} \]

\[ \lambda_k = \min_{x \perp v_1, \ldots, v_{k-1}} \frac{x^T L x}{x^T x} \]

\[ v_k = \arg \min_{x \perp v_1, \ldots, v_{k-1}} \frac{x^T L x}{x^T x} \]
The first eigenvalue

\[ \lambda_1 = \min_{x \neq 0} \frac{x^T Lx}{x^T x} \]

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

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

We find \( \lambda_1 = 0 \) and \( v_1 = 1 \)
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
The second eigenvalue

\[ \lambda_2 > 0 \quad \text{if and only if G is connected} \]

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

![Graphs](image.png)
The second eigenvalue

\[ \lambda_2 > 0 \quad \text{if and only if G is connected} \]

Proof: if G is connected,

\[ x \perp 1 \quad \text{means} \quad \sum_a x(a) = 0 \]

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

\[ x(a) < x(b) \quad \text{and so} \quad (x(a) - x(b))^2 > 0 \]
The second eigenvalue

\[ \lambda_2 > 0 \text{ if and only if } G \text{ is connected} \]

Proof: if \( G \) is connected,

\[ x \perp \mathbf{1} \text{ means } \sum_a x(a) = 0 \]

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

\[ x(a) < x(b) \text{ and so } (x(a) - x(b))^2 > 0 \]
The second eigenvalue

\[ \lambda_2 > 0 \] if and only if G is connected

Fiedler (‘73) called \( \lambda_2 \)
“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. $\lambda_2$ is big if and only if $\text{G}$ does not have good clusters.

2. If $\lambda_2$ is small, can use $\nu_2$ to find a good cluster.
Cheeger’s Inequality  [Cheeger ‘70]

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

1. $\lambda_2$ 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]
[Alon-Milman ‘85, Jerrum-Sinclair ‘89, Diaconis-Stroock ‘91]

1. $\lambda_2$ is big if and only if $G$ does not have good clusters.

2. If $\lambda_2$ is small, can use $\nu_2$ to find a good cluster.

*In a moment…*
Spectral Graph Drawing [Hall ‘70]
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
The Airfoil Graph, spectral coordinates
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 \( a \)

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

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

For planar graphs:

\( \lambda_2 \leq 8d/n \) \quad [S-Teng '96]

\( \lambda_3 \leq O(d/n) \) \quad [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]

\[ S = \{ a : v_2(a) \leq t \} \text{ for some } t \]
Spectral Graph Partitioning
[Donath-Hoffman ‘72, Barnes ‘82, Hagen-Kahng ‘92]

Cheeger’s Inequality says there is a \( t \) so that

\[
S = \{ a : v_2(a) \leq t \} \text{ for some } t
\]

\[\Phi(S) \leq \sqrt{2d\lambda_2}\]
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.
Maximum flow problem

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

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

Standard approach: incrementally add flow paths
Maximum flow problem

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Standard approach: incrementally add flow paths
Maximum flow problem

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

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.

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![Graph with node labels and flow values](image-url)
Maximum flow problem, electrical approach

[Christiano-Kelner-Madry-S-Teng ‘11]

1. Try the electrical flow.
2. Increase resistance when too much flow
Maximum flow problem, electrical approach

[Christiano-Kelner-Madry-S-Teng ‘11]

1. Try the electrical flow.
2. Increase resistance when too much flow
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 $\epsilon$-approximation of $G$ if

for all $x$

\[
\frac{1}{1 + \epsilon} \leq \frac{x^T L_H x}{x^T L_G x} \leq 1 + \epsilon
\]
Approximating Graphs

A graph $H$ is an $\epsilon$-approximation of $G$ if for all $x$

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

To solve linear equations quickly, approximate $G$ by a simpler graph $H$.
Approximating Graphs

A graph $H$ is an $\epsilon$-approximation of $G$ if for all $x$

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

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

A graph $H$ is an $\epsilon$-approximation of $G$ if

for all $x$

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

Theorem [Batson-S-Srivastava ‘09]

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

A graph $H$ is an $\epsilon$-approximation of $G$ if

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

for all $x$.

Theorem [Batson-S-Srivastava ‘09]
Every graph $G$ has an $\epsilon$-approximation $H$ with

$$|V| \frac{(2 + \epsilon)^2}{\epsilon^2}$$

edges

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”