

# Embedding and Spectrum of Graphs

Ali Shokoufandeh,

Department of Computer Science, Drexel University

# Overview

Approximation Algorithms

Geometry of Graphs and Graphs Encoding the Geometry

Spectral Graph Theory

# Algorithmic Graph Theory:

- **Objective:** Designing efficient combinatorial methods for solving decision or optimization problems.
  - Runs in polynomial number of steps in terms of size of the graph;  $n=|V(G)|$  and  $m=|E(G)|$ .
  - Optimality of solution.
- **Bad news:** most of the combinatorial optimization problems involving graphs are computationally intractable:
  - traveling salesman problem, maximum cut problem, independent set problem, maximum clique problem, minimum vertex cover problem, maximum independent set problem, multidimensional matching problem,...

# Algorithmic Graph Theory:

- **Dealing with the intractability:**
  - Bounded approximation algorithms
  - Suboptimal heuristics.

# Algorithmic Graph Theory:

## Bounded approximation algorithms

□ Example: Vertex cover problem:

□ A *vertex cover* of an undirected graph  $G=(V,E)$  is a subset  $V'$  of  $V$  such that if  $(u,v)$  is an edge in  $E$ , then  $u$  or  $v$  (or both) belong to  $V'$ .

# Algorithmic Graph Theory:

## Bounded approximation algorithms

□ Example: Vertex cover problem:

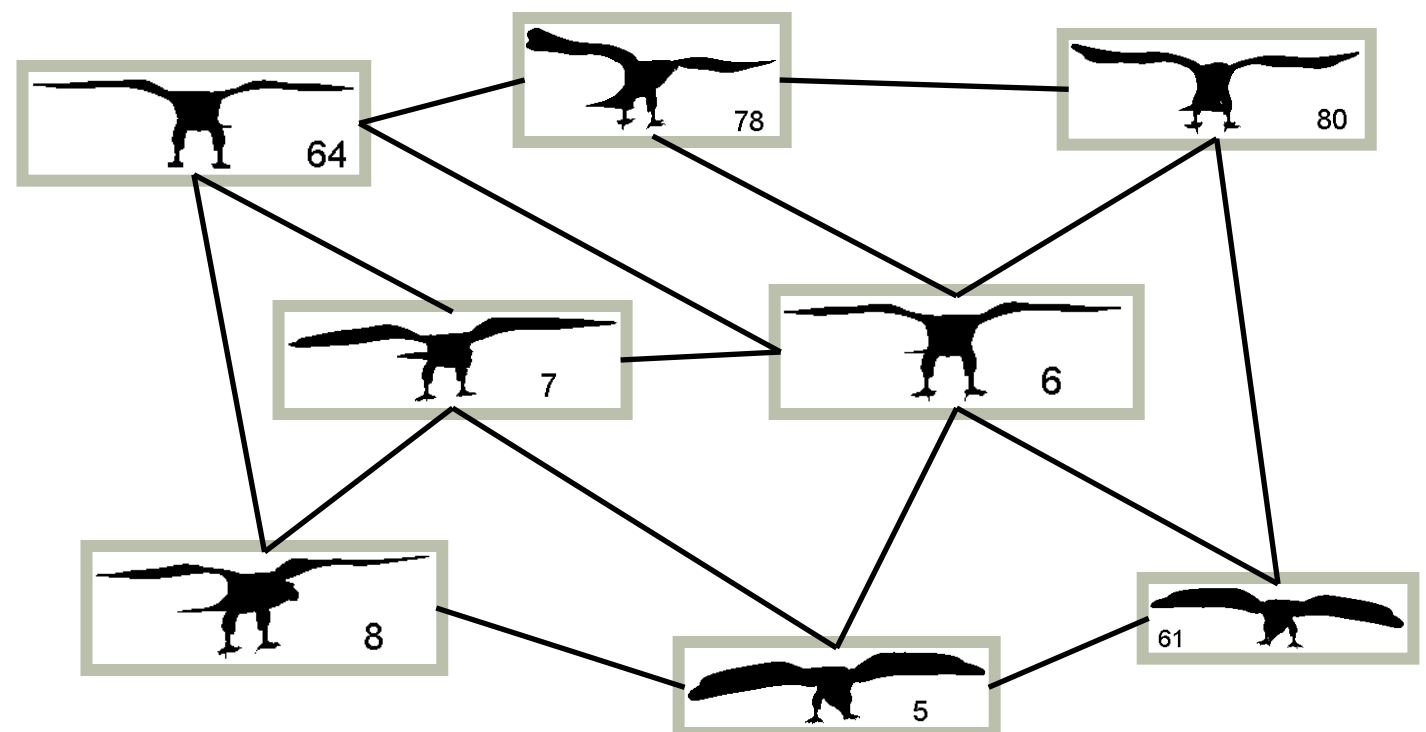
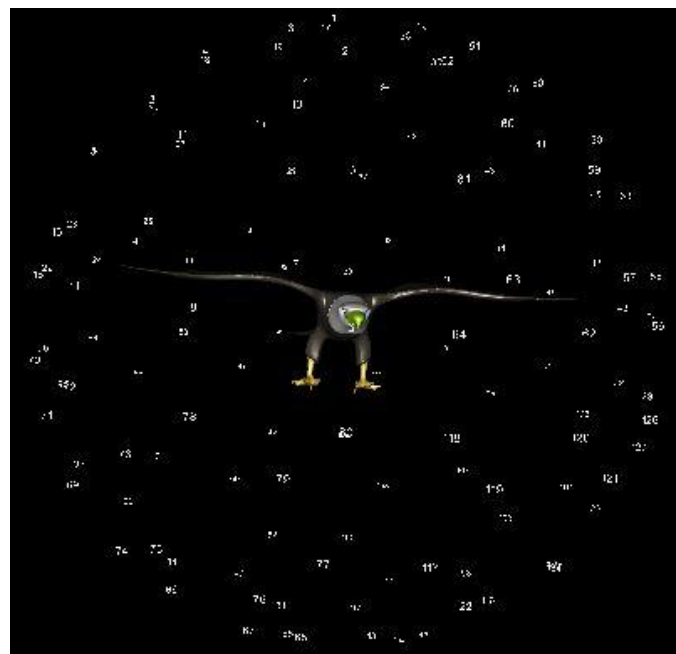
- A ***vertex cover*** of an undirected graph  $G=(V,E)$  is a subset  $V'$  of  $V$  such that if  $(u,v)$  is an edge in  $E$ , then  $u$  or  $v$  (or both) belong to  $V'$ .
- The ***vertex cover problem*** is to find a vertex cover of minimum size in a given undirected graph.

# Algorithmic Graph Theory:

## Bounded approximation algorithms

Example: Vertex cover problem:

- A **vertex cover** of an undirected graph  $G=(V,E)$  is a subset  $V'$  of  $V$  such that if  $(u,v)$  is an edge in  $E$ , then  $u$  or  $v$  (or both) belong to  $V'$ .
- The **vertex cover problem** is to find a vertex cover of **minimum** size in a given undirected graph.

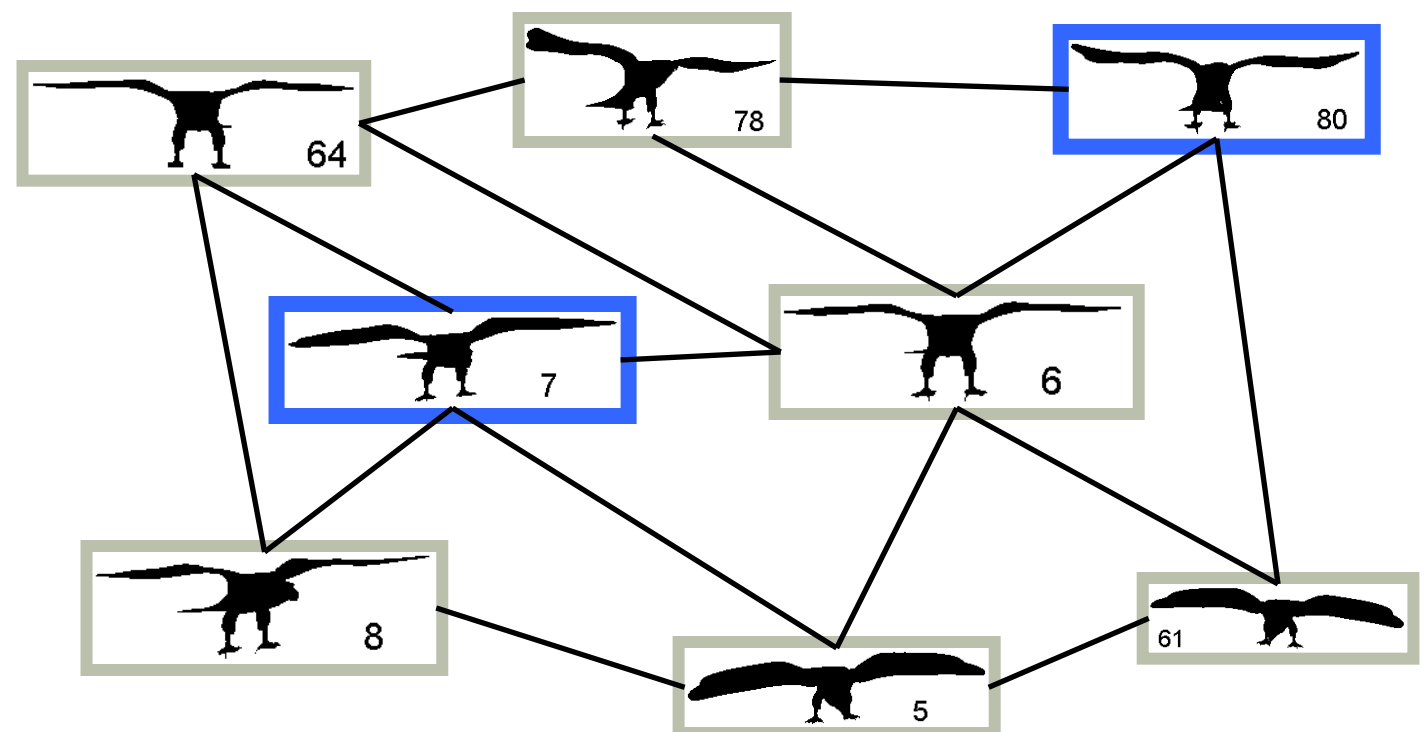
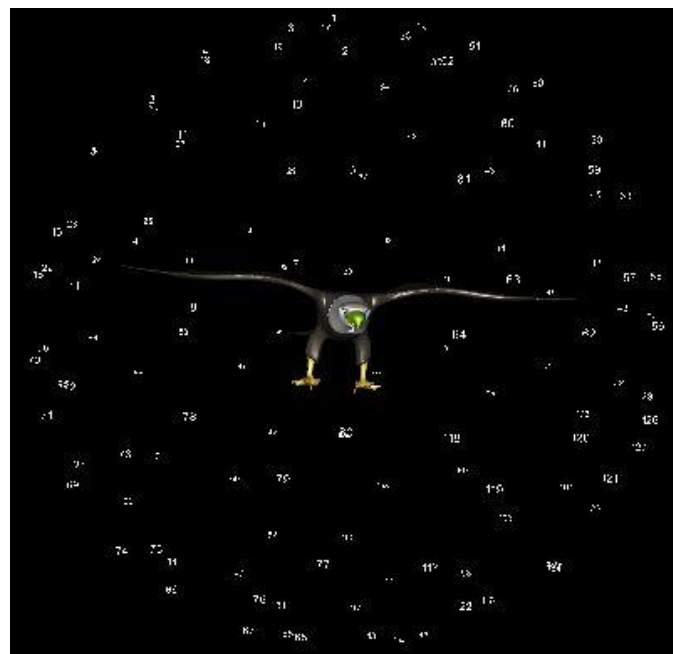


# Algorithmic Graph Theory:

## Bounded approximation algorithms

Example: Vertex cover problem:

- A **vertex cover** of an undirected graph  $G=(V,E)$  is a subset  $V'$  of  $V$  such that if  $(u,v)$  is an edge in  $E$ , then  $u$  or  $v$  (or both) belong to  $V'$ .
- The **vertex cover problem** is to find a vertex cover of **minimum** size in a given undirected graph.





# Algorithmic Graph Theory:

## Bounded approximation algorithms

□ Example: Vertex cover problem:

- A ***vertex cover*** of an undirected graph  $G=(V,E)$  is a subset  $V'$  of  $V$  such that if  $(u,v)$  is an edge in  $E$ , then  $u$  or  $v$  (or both) belong to  $V'$ .
- The size of a vertex cover is the number of vertices in it.
- The ***vertex cover problem*** is to find a vertex cover of **minimum** size in a given undirected graph.
- We call such a vertex cover an ***optimal vertex cover***.
- The vertex cover problem was shown to be NP-complete.

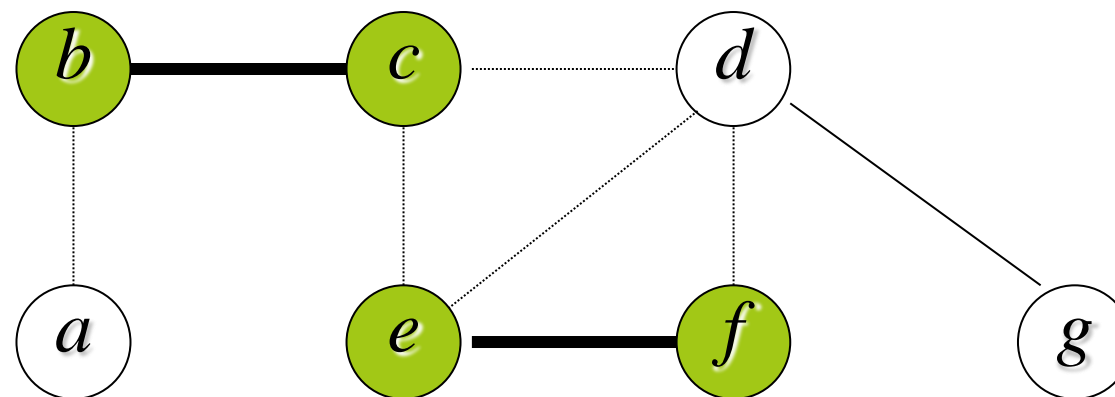
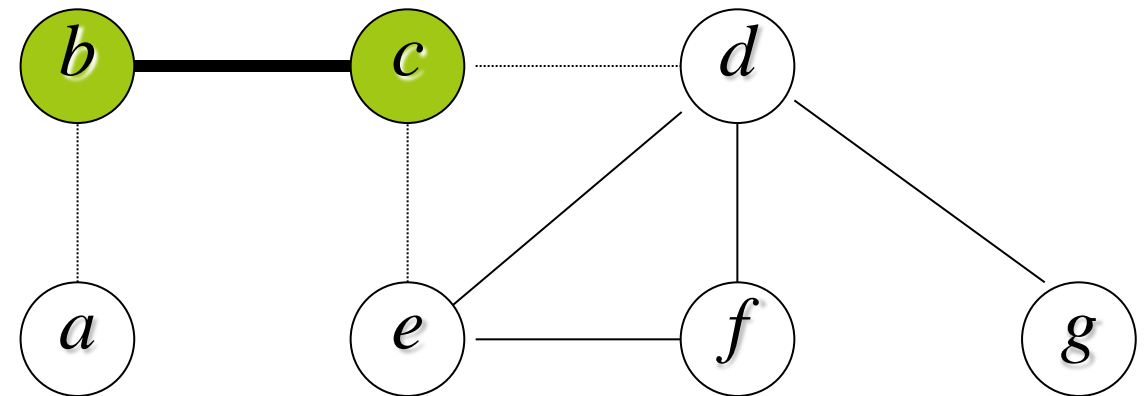
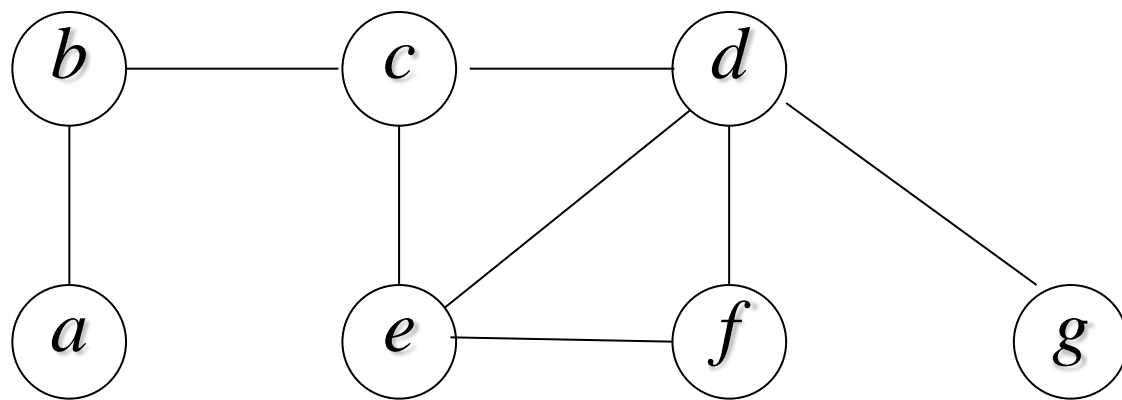
# Algorithmic Graph Theory:

## Vertex cover problem:

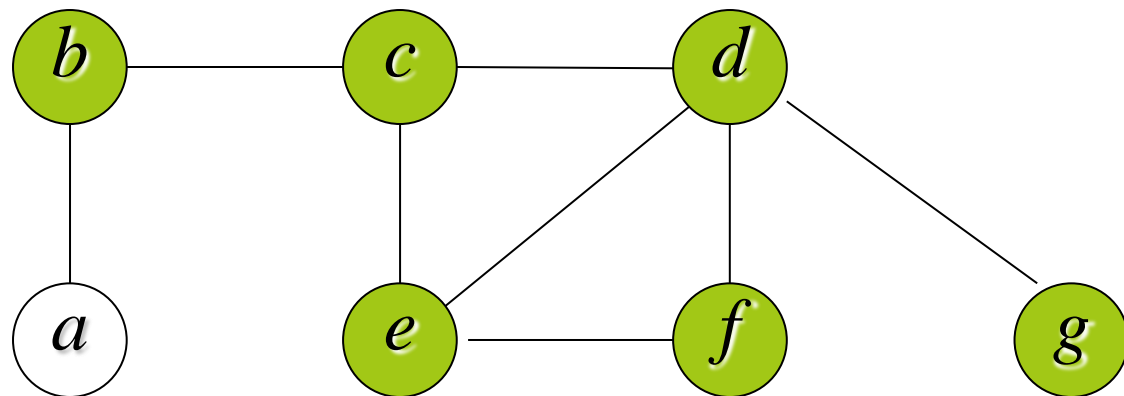
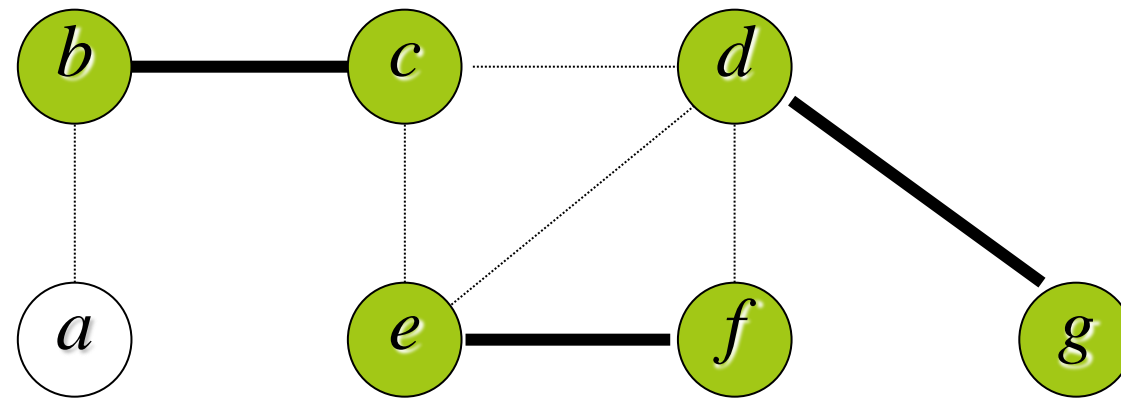
- The following approximation algorithm takes as input an undirected graph  $G$  and returns a vertex cover whose size is guaranteed no more than twice the size of optimal vertex cover:

1.  $C \leftarrow \emptyset$
2.  $E' \leftarrow E[G]$
3. While  $E' \neq \emptyset$  do
4.    Let  $(u, v)$  be an arbitrary edge in  $E'$
5.     $C \leftarrow C \cup \{u, v\}$
6.    Remove from  $E'$  every edge incident on either  $u$  or  $v$
7. Return  $C$

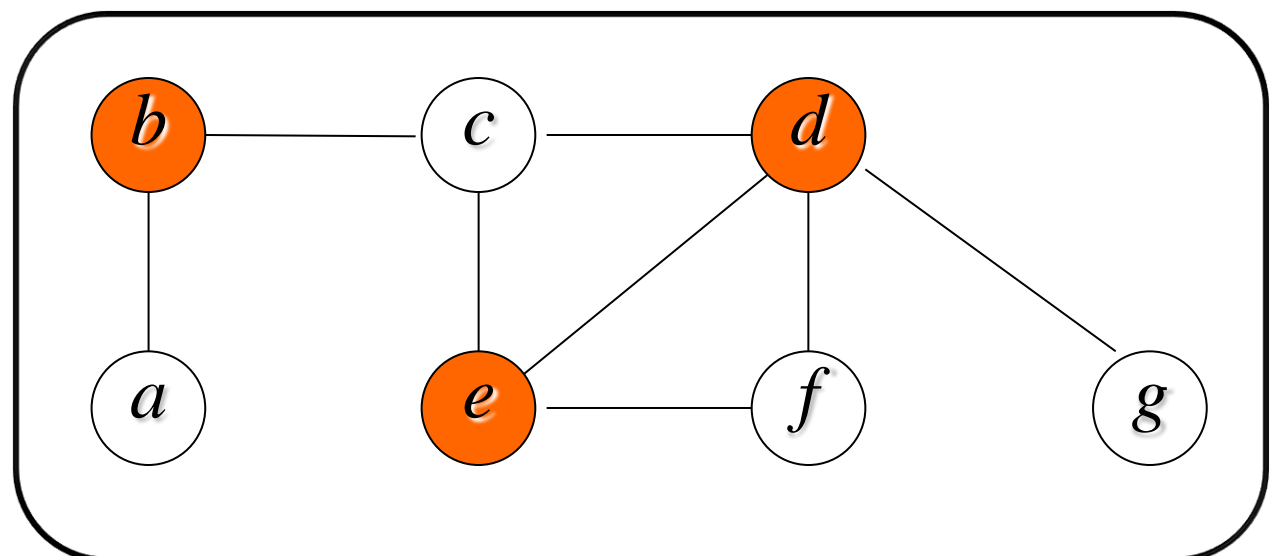
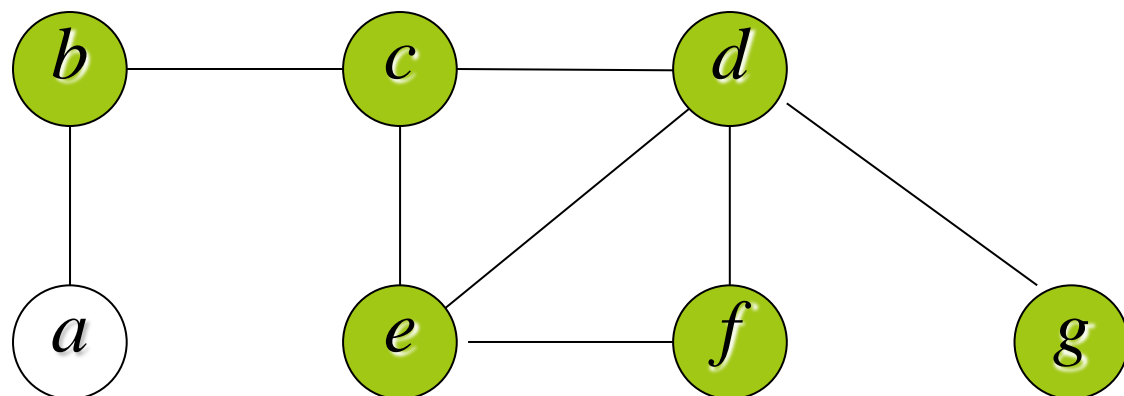
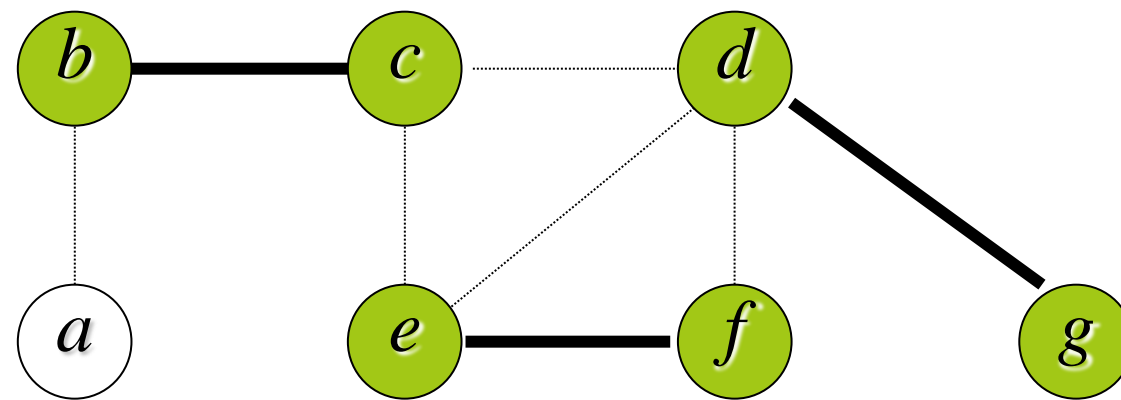
# Algorithmic Graph Theory:



# The Vertex Cover Problem



# The Vertex Cover Problem



# Algorithmic Graph Theory:

**Theorem:** Approximate vertex cover has a ratio bound of 2.

□ ***Proof:***

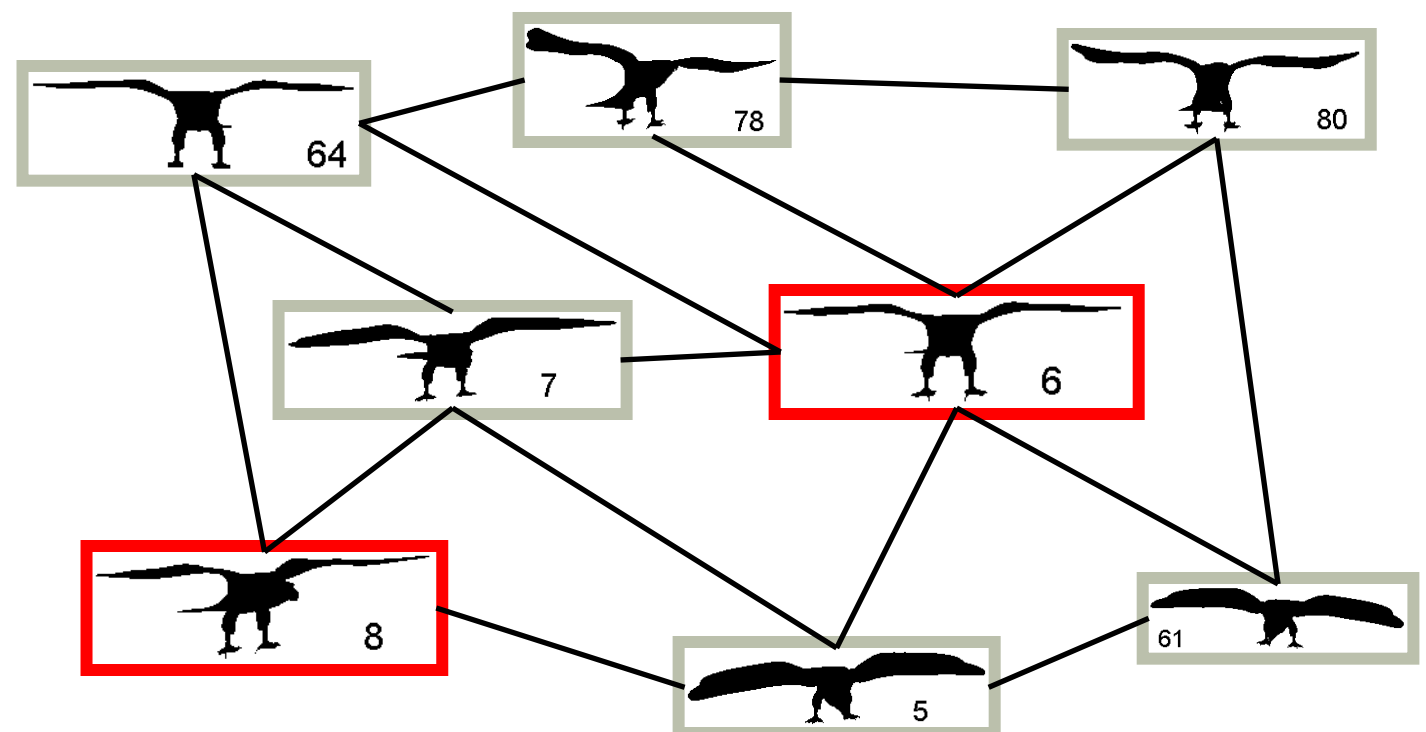
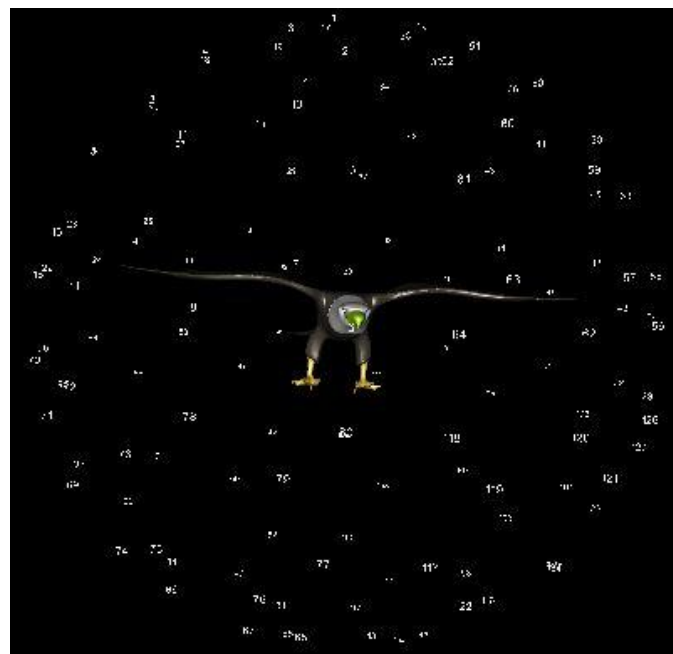
- It is easy to see that  $C$  is a vertex cover.
- To show that the size of  $C$  is twice the size of optimal vertex cover.
- Let  $A$  be the set of edges picked in line 4 of algorithm.
- No two edges in  $A$  share an endpoint, therefore each new edge adds two new vertices to  $C$ , so  $|C|=2|A|$ .
- Any vertex cover should cover the edges in  $A$ , which means at least one of the end points of each edge in  $A$  belongs to  $C^*$ .
- So,  $|A| \leq |C^*|$ , which will imply the desired bound.

# Algorithmic Graph Theory:

## Bounded approximation algorithms

Example: Vertex cover problem:

- A **vertex cover** of an undirected graph  $G=(V,E)$  is a subset  $V'$  of  $V$  such that if  $(u,v)$  is an edge in  $E$ , then  $u$  or  $v$  (or both) belong to  $V'$ .
- The **vertex cover problem** is to find a vertex cover of **minimum** size in a given undirected graph.



# Overview

**Geometry of Graphs and Graphs Encoding the Geometry**

Spectral Graph Theory

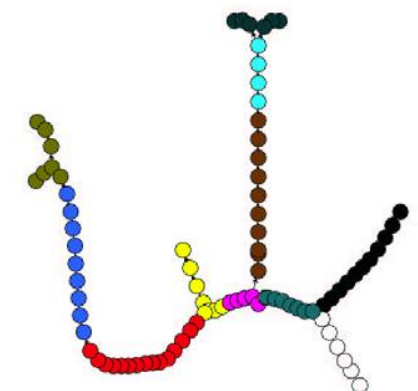
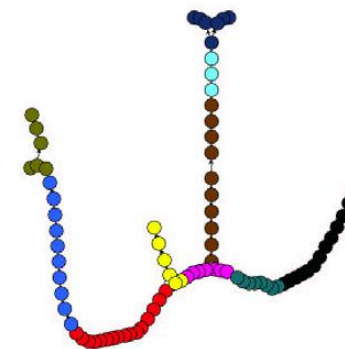
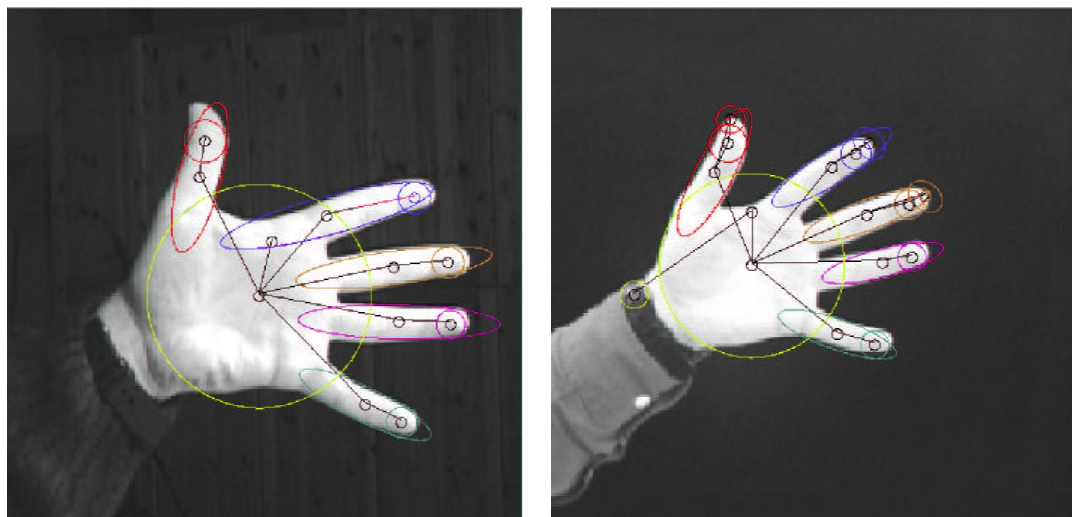


# Motivation:

- In some scenarios geometrical problem in a finite metric space is easier to solve (approximate) than the corresponding combinatorial or optimization problem.
- Example: Many-to-many graph matching.

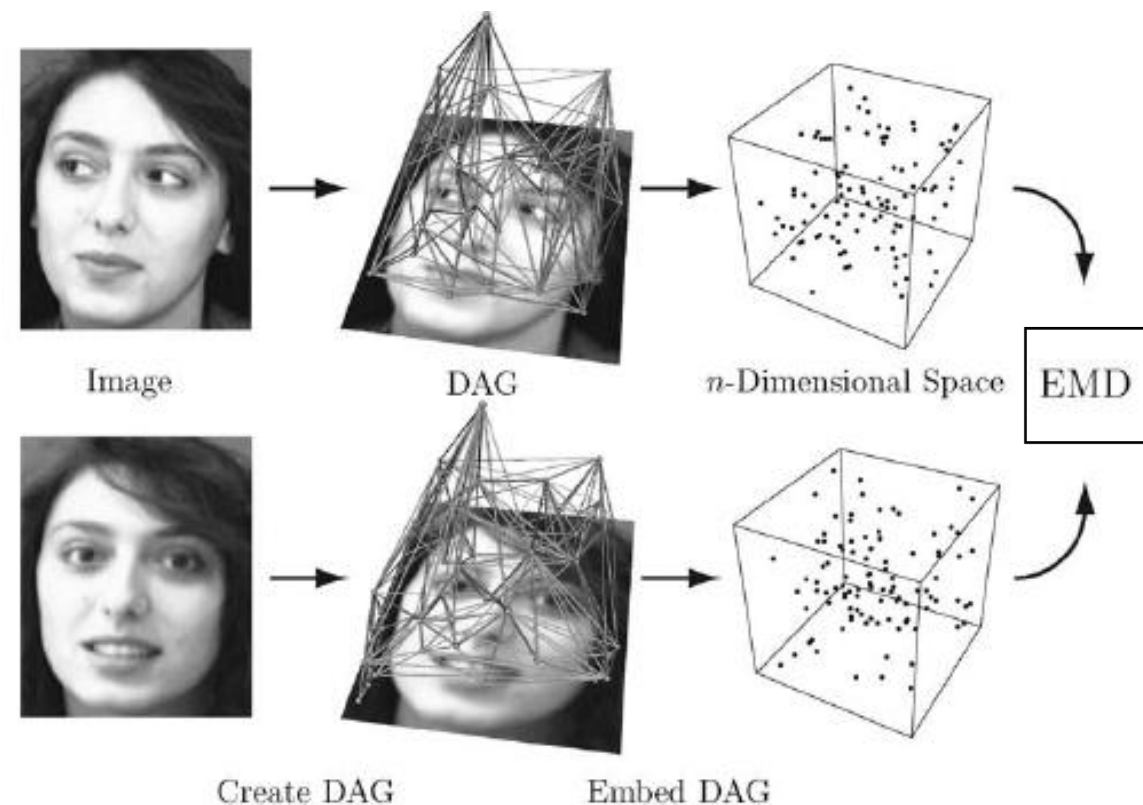
# Motivation:

- In some scenarios geometrical problem in a finite metric space is easier to solve (approximate) than the corresponding combinatorial or optimization problem.
- Example: Many-to-many graph matching.



# Motivation:

- In some scenarios geometrical problem in a finite metric space is easier to solve (approximate) than the corresponding combinatorial or optimization problem.
- Example: Many-to-many graph matching.



# Some Formalities:

**(semi) metric**  $(M, \rho)$ :  $M$  a (finite) set of points,  $\rho$  a distance function satisfying for all  $x, y, z$  in  $M$ :

- ▣  $\rho(x, x) = 0$ ,
- ▣  $\rho(x, y) = \rho(y, x)$ ,
- ▣  $\rho(x, z) \leq \rho(x, y) + \rho(y, z)$ .

**Embedding**: a mapping  $f: (M, \rho) \rightarrow (H, \nu)$  of a metric space  $M$  into a host metric space  $H$ , that (possibly) preserves the geometry (distances) of  $M$ .

**Distortion of embedding  $f$** : the least  $K \geq 1$  for which exists  $C > 0$  such that for all  $x, y$  in  $M$ :

$$C \times \rho(x, y) \leq \nu(x, y) \leq K \times C \times \rho(x, y)$$

# Non-embedability:

- **Given:**  $\rho$  the (Shortest Path) metric of the graph  $C_4$ , a cycle on four nodes.
- **Question:** Is there an isometric embedding of  $C_4$  in Euclidean space?

# Non-embedability:

- **Given:**  $\rho$  the (Shortest Path) metric of the graph  $C_4$ , a cycle on four nodes.
- **Question:** Is there an isometric embedding of  $C_4$  in Euclidean space?
- **No:**
  - Denote the vertices on the  $C_4$  by  $a_1, \dots, a_4$ .
  - Suppose an *isometric* embedding exists.
  - Note that  $\rho(a_1, a_3) = \rho(a_1, a_2) + \rho(a_2, a_3)$ , hence the triangle inequality holds with equality, which means (for Euclidean spaces) that  $f(a_2)$  is in the middle of the segment  $[f(a_1), f(a_3)]$ .

# Non-embedability:

- **Given:**  $\rho$  the (Shortest Path) metric of the graph  $C_4$ , a cycle on four nodes.
- **Question:** Is there an isometric embedding of  $C_4$  in Euclidean space?
- **No:**
  - Denote the vertices on the  $C_4$  by  $a_1, \dots, a_4$ .
  - Suppose an *isometric* embedding exists.
  - Note that  $\rho(a_1, a_3) = \rho(a_1, a_2) + \rho(a_2, a_3)$ , hence the triangle inequality holds with equality, which means (for Euclidean spaces) that  $f(a_2)$  is in the middle of the segment  $[f(a_1), f(a_3)]$ .
  - Analogously,  $f(a_4)$  is in the middle of the segment  $[f(a_1), f(a_3)]$ .
  - Hence  $f(a_2) = f(a_4)$ .  $\rightarrow \leftarrow$

# Non-embedability:

- **Given:**  $\rho$  the (Shortest Path) metric of the graph  $C_4$ , a cycle on four nodes.
- **Question:** Is there an isometric embedding of  $C_4$  in Euclidean space?
  - **No.**
- Embedding of  $C_4$  as a square in the plane is the best embedding in Hilbert space, (distortion =  $\sqrt{2}$ ).



# Example Application:

## Sparsest Cut and Flux Minimization Problem:

- A cut in graph  $G = (V, E)$  is a partition of  $V$  into two nonempty subsets  $A$  and  $B = V - A$ .
- The density or flux of the cut  $(A, B)$  is

$$\Upsilon(A, B) = \frac{e(A, B)}{|A| \times |B|}$$

where  $e(A, B)$  is the number (or the weight) of edges crossing the cut.

- The sparsity of an  $(A, B)$ -cut will be defined as

$$\alpha(A, B) = \frac{e(A, B)}{\min(|A|, |B|)}$$

# Example Application:

## Sparsest Cut and Flux Minimization Problem:

□ It is not hard to see that

$$\frac{a(A, B)}{|V|} \leq \Upsilon(A, B) \leq \frac{2 \times a(A, B)}{|V|}$$

# Example Application:

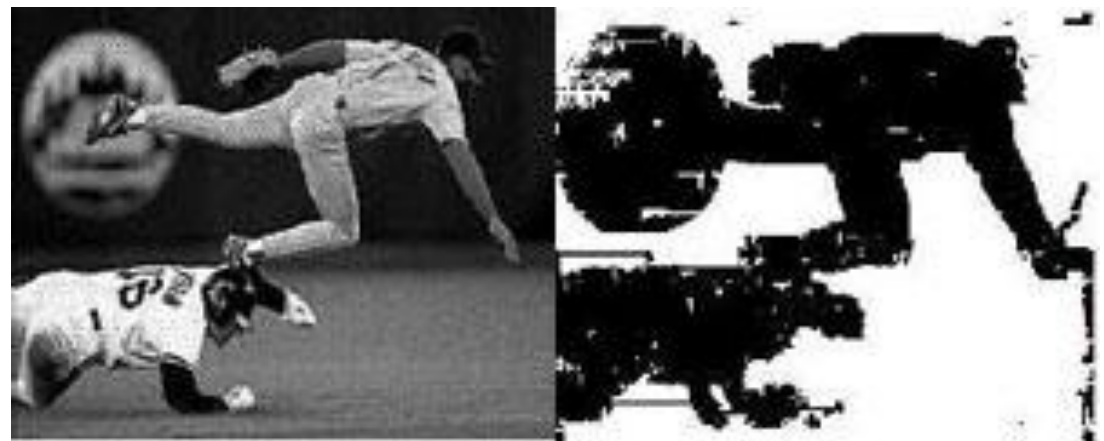
## Sparsest Cut Problem:

- In sparsest cut problem we look for a cut of the smallest possible density.
- This problem is known to be **NP**-hard.
- As optimization problems this are **minimization** problems and intractable.

# Example Application:

## Sparsest Cut Problem:

- In sparsest cut problem we look for a cut of the smallest possible density.
- This problem is known to be **NP**-hard.
- As optimization problems this are **minimization** problems and intractable.



Shi and Malik, 1999

# Example Application:

Flux Minimization Problem:

■ The flux problem can be formulated as embedding:

Find a mapping  $\phi: V \rightarrow \{0,1\}$  that minimizes:

$$\frac{\sum_{(u,v) \in E} |f(u) - f(v)|}{\sum_{(u,v) \in V^2} |f(u) - f(v)|}$$

# Example Application:

**Flux minimization problem:**

$$\min_f \frac{\sum_{(u,v) \in E} |f(u) - f(v)|}{\sum_{(u,v) \in V^2} |f(u) - f(v)|}$$

■ Simple modification of the flux formulation:

- letting  $d_{u,v} = |\phi(u) - \phi(v)|$ ,
- Setting denominator  $\sum_{(u,v) \in V^2} |f(u) - f(v)| \approx 1$
- Enforcing triangle inequality  $d_{u,v} \leq d_{u,w} + d_{w,v}$

# Example Application:

## Flux minimization problem:

□ Simple modification of the flux formulation:

- letting  $d_{u,v} = |\phi(u) - \phi(v)|$ ,
- Setting denominator  $\hat{a}_{(u,v)} = |f(u) - f(v)|^3$
- Enforcing triangle inequality  $d_{u,v} \leq d_{u,w} + d_{w,v}$
- Relax the  $d_{u,v} \in \{0,1\}$  and solve:

$$\begin{aligned}
 \min \quad & \sum_{(u,v) \in E} \hat{a}_{(u,v)} d_{u,v} \\
 \text{s.t.} \quad & \sum_{(u,v) \in V^2} \hat{a}_{(u,v)} d_{u,v}^3 = 1 \\
 & d_{u,v} \leq d_{u,w} + d_{w,v} \\
 & 0 \leq d_{u,v} \leq 1
 \end{aligned}$$

# Example Application:

## Now what?

- The solution of LP gives us a metric  $(V, d)$ .
- We can use Bourgain's theorem:

*For any metric space  $(V, d)$  with  $|V|=n$  there is an embedding into  $R^{(\log n)^2}$  under  $L_1$  with  $O(\log n)$  distortion. And we can construct this embedding in poly-time using a randomized algorithm.*



# Example Application:

**Now what?**

□ The solution of LP gives us a metric  $(V, d)$ .

□ We can use Bourgain's theorem:

*For any metric space  $(V, d)$  with  $|V|=n$  there is an embedding into  $R^{(\log n)^2}$  under  $L_1$  with  $O(\log n)$  distortion. And we can construct this embedding in poly-time using a randomized algorithm.*

□ Suppose  $\omega: V \rightarrow R^{(\log n)^2}$  is such an embedding, we have

$$d_{u,v} \leq |\omega(u) - \omega(v)| \leq d_{u,v} \times \log^2 n$$

# Example Application:

**Now what?**

- Form the cut  $S_{i,j} = (A_{i,j}, B_{i,j})$ , for  $j$  in  $\{1, \dots, n-1\}$  as follows:
  - Fix a coordinate  $i$  in  $\{1, \dots, \log^2 n\}$ .
  - Order the vector with respect to their  $i$ -th coordinate  $\omega_i(u)$
  - Take the first  $j$  points as  $A_{i,j}$
  - Take the other  $n-j$  points as  $B_{i,j}$

# Example Application:

**Now what?**

- Form the cut  $S_{i,j} = (A_{i,j}, B_{i,j})$ , for  $j$  in  $\{1, \dots, n-1\}$  as follows:
  - Fix a coordinate  $i$  in  $\{1, \dots, \log^2 n\}$ .
  - Order the vector with respect to their  $i$ -th coordinate  $\omega_i(u)$
  - Take the first  $j$  points as  $A_{i,j}$
  - Take the other  $n-j$  points as  $B_{i,j}$
- This will result in  $n \times \log^2 n$  cuts of the form  $S_{i,j}$ .
- Choose the one that gives the minimum flux value.
- **Theorem:** The procedure described above generates a cut within a factor of  $O(\log n)$  to the optimal in poly-time.

# Overview

Geometry of Graphs and Graphs Encoding the Geometry

**Spectral Graph Theory**

# Introduction:

- Spectral graph theory is a branch of Algebraic graph Theory (the study of matrices associated with a graph).
- Spectral graph theory deals with studying spectral operators associated with a graph:
  - For an  $n \times n$  matrix  $A$  having a basis of right-eigenvalues  $v_1, \dots, v_n$  means:

$$Av_i = \lambda_i v_i$$

- Assuming  $x = c_1 v_1 + \dots + c_n v_n$ , as an operator, the behavior of  $A$  on vector  $x$  can be expressed as

$$A^k x = \sum_i c_i A^k v_i = \sum_i c_i \lambda_i^k v_i$$

# Notations:

- Adjacency operator:

$$A_G(i, j) = \begin{cases} 1 & \text{if } (i, j) \in E(G) \\ 0 & \text{Otherwise} \end{cases}$$

- Observer that for a vector  $x$ :

$$(A_G x)(u) = \sum_{v: (u, v) \in E} x(v)$$

- Define  $d(v) = |\{u \mid (u, v) \in E(G)\}|$  then degree matrix

$$D_G(u, v) = \begin{cases} d(u) & \text{if } (u, v) \in E(G) \\ 0 & \text{Otherwise} \end{cases}$$

# Notations:

- Using Degree matrix

$$D_G(u, v) = \begin{cases} d(u) & \text{if } (u, v) \in E(G) \\ 0 & \text{Otherwise} \end{cases}$$

- Diffusion matrix operator:

$$W_G = A_G D_G^{-1}$$

- The action of this operator on a vector  $x$ :

$$(W_G x)(u) = \sum_{v: (u, v) \in E} x(v) / d(u)$$

# Quadratic forms:

- Laplacian forms:

$$x^T L_G x = \sum_{(u,v) \in E} L_G(u,v) \times (x(u) - x(v))^2$$

- **Motivation:**

- measures the smoothness of walk denoted by function  $x$  (its value is small if  $x$  does not change dramatically along each edge).
- As a matrix operator:

$$L_G = D_G - A_G$$

- Normalized version

$$N_G = D^{-1/2} L_G D^{-1/2} = I - D^{-1/2} A_G D^{-1/2}$$



# Courant-Fisher Theorem:

- The Rayleigh quotient of a nonzero vector  $x$  with respect to symmetric matrix  $A$ :

$$\frac{x^T A x}{x^T x}$$

- **Theorem:** Let  $A$  be a symmetric matrix with spectrum  $\alpha_1 \geq \dots \geq \alpha_n$ .  
Then

$$a_k = \max_{\substack{S \subseteq \mathbb{R}^n \\ \dim(S)=k}} \min_{\substack{x \in S \\ x \neq 0}} \frac{x^T A x}{x^T x} = \min_{\substack{T \subseteq \mathbb{R}^n \\ \dim(T)=n-k+1}} \max_{\substack{x \in T \\ x \neq 0}} \frac{x^T A x}{x^T x}$$

# Low-rank Approximation:

- Eigenvalues and eigenvectors provide low-rank approximation of a matrix.

- Recall, for matrix  $A$  with spectrum  $\alpha_1 \geq \dots \geq \alpha_n$ :

$$A = \sum_i \alpha_i v_i v_i^T$$

- Consequence of Courant-Fischer:

- For every  $k$ , the best approximation of  $A$  by a rank  $k$  matrix can be obtained by

$$\hat{A} = \sum_{i=1}^k \alpha_i v_i v_i^T$$

- i.e

$$\hat{A} = \arg \min_{\text{rank}(B)=k} \|A - B\|_F$$

# Notes:

- The all-ones vector is an eigenvector of  $L_G$ .
- Let  $\alpha_1 \geq \dots \geq \alpha_n$  denote the spectrum of  $A_G$ , then:

$$\bar{d}(G) \leq \alpha_1 \leq D(G).$$

- The all-ones is an eigenvector of  $A_G$  only if  $G$  is a regular graph.
- Multiplicity of  $0$  eigenvalue of  $L_G$  is the number of connected components of  $G$ .
- Let  $\lambda_1 \geq \dots \geq \lambda_n$  denote the spectrum of  $L_G$ , then:

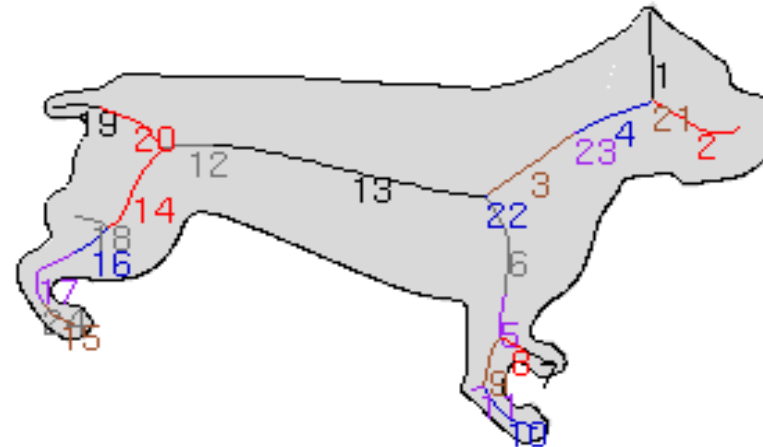
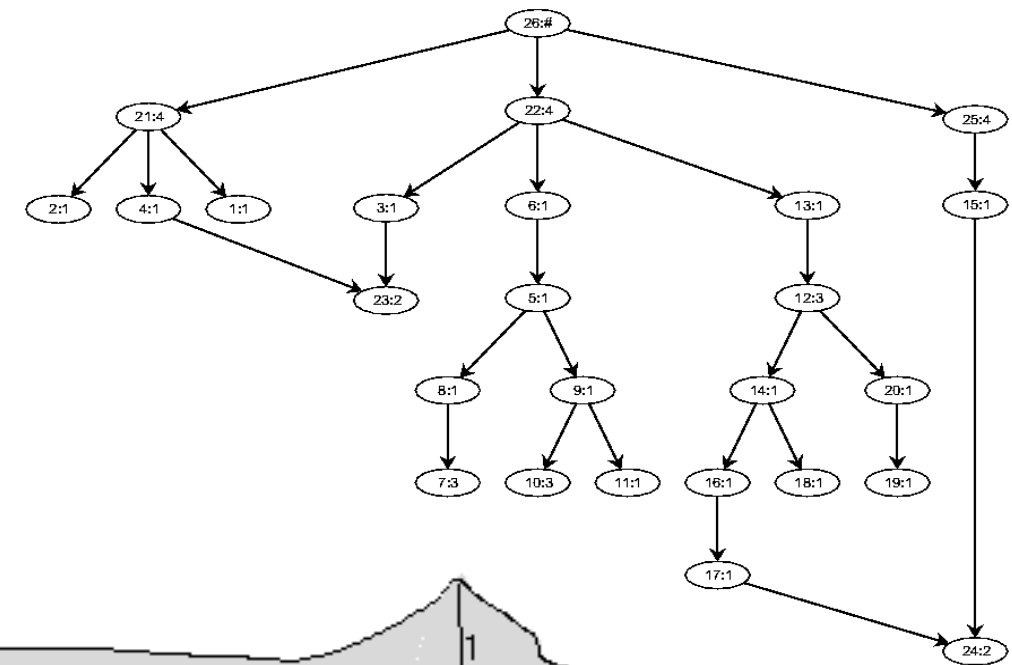
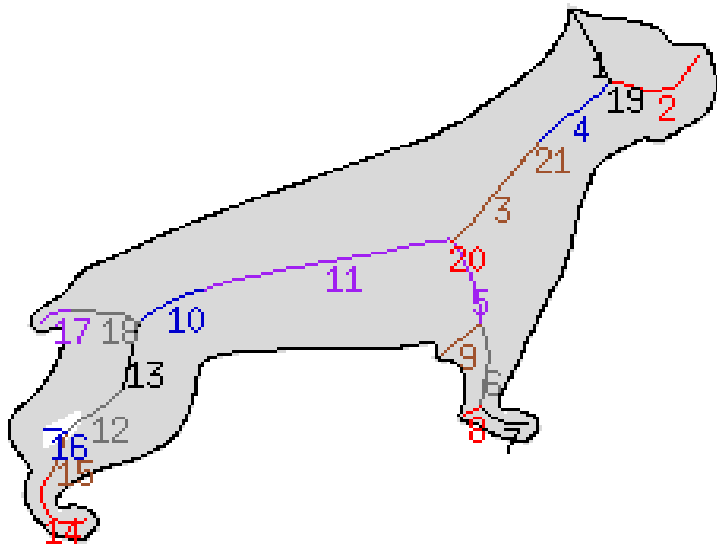
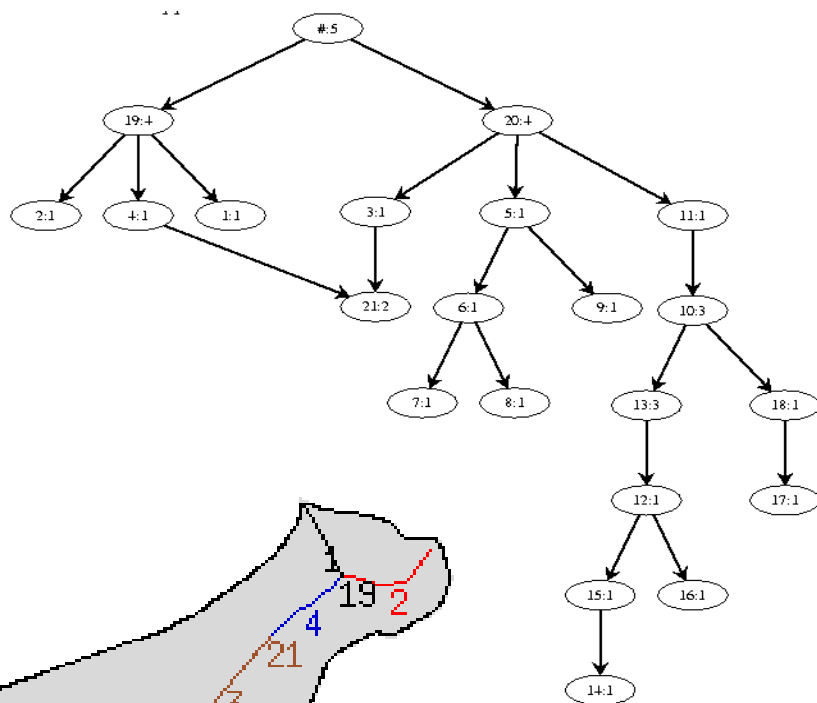
$$\lambda_1 \leq 2 \times D(G).$$

- If  $\alpha_1 = -\alpha_n$  only if  $G$  is a bipartite graph.

# Matching Spectral Abstractions of Graph Structures

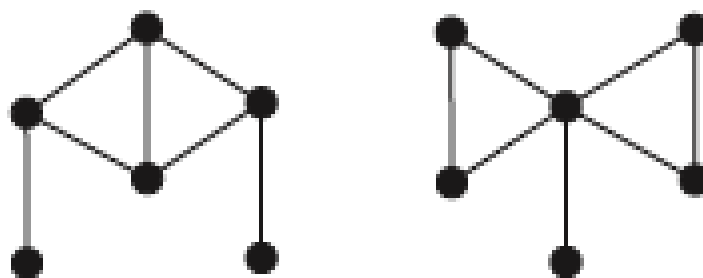
- Image features and their relations can be conveniently represented by labeled graphs.
- When features are multi-scale, or when part/whole relations exist between features, resulting graphs can be represented as directed acyclic graphs.
- Object recognition can therefore be formulated as hierarchical graph matching.
- Using spectral graph theory, we embed discrete graphs into low-dimensional continuous spaces.

# Matching Spectral Abstractions of Graph Structures



# The Eigenspace and Isomorphism

- If two graphs have different spectra (equivalently, different characteristic polynomials) of the adjacency matrix, then they are not isomorphic
- However, non-isomorphic graphs can be co-spectral!
- But, are they unique? No, but co-spectral graphs are not that common.



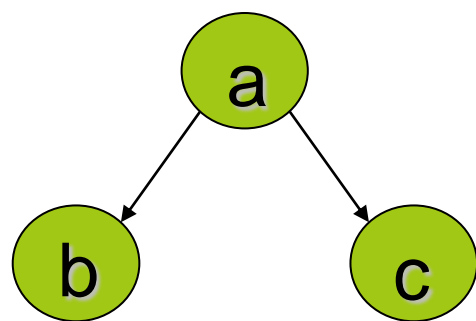
$$p(x) = x^6 - 7x^4 - 4x^3 + 7x^2 + 4x - 1$$

# The Eigenspace and Isomorphism

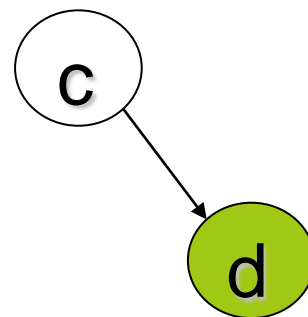
- Clearly, isomorphic graphs must have the same adjacency and Laplacian spectrum (i.e., Laplacian characteristic polynomial)
- **Bad news:** non-isomorphic graphs can be adjacency or Laplacian cospectral
- [Schwenk 73], [McKay 77] For almost all trees  $T$  there is a non-isomorphic tree  $T'$  that has both the same adjacency spectrum and the same Laplacian spectrum
- **Idea:**
  - Use the spectrum of all subgraphs associated with a graph for its characterization.

# Perturbation

- How robust is the spectrum under noise and minor structural perturbation?

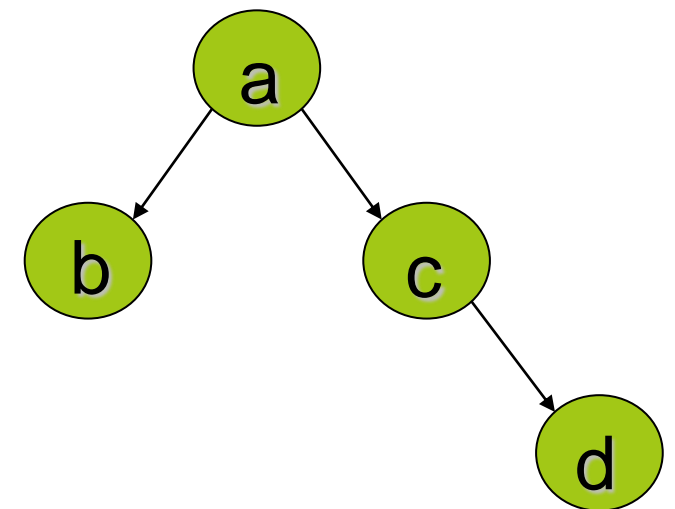


G (original)



E (noise)

=



H (perturbed)

	a	b	c	
a	0	1	1	0
b	-1	0	0	0
c	-1	0	0	0
	0	0	0	0

$\Psi(A_G)$

+

	a	b	c	d
a	0	0	0	0
b	0	0	0	0
c	0	0	0	1
d	0	0	-1	0

$A_E$

=

	a	b	c	
a	0	1	1	0
b	-1	0	0	0
c	-1	0	0	1
	0	0	-1	0

$A_H$



# Perturbation:

- Let  $S$  denote a subset of vertices  $V(G)$ ,  $A(X)$ , the induced sub-matrix corresponding to set  $X$ , and  $A(X, Y)$  the adjacency matrix between sets  $X$  and  $Y$ .

- We have

$$A(G) = \begin{pmatrix} A(S) & 0 \\ 0 & A(V-S, S) \end{pmatrix}$$

- How the eigenvalues of  $A$  are related to those of the other matrices?

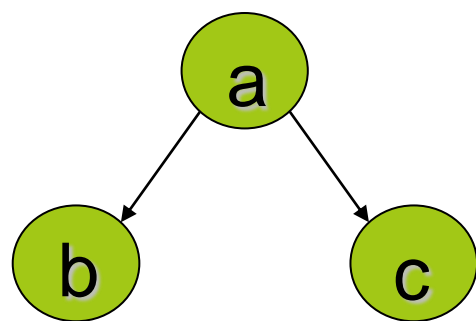
# Perturbation:

- Let  $X$  and  $Y$  denote two symmetric matrices with eigenvalues  $\alpha_1 \geq \dots \geq \alpha_n$  and  $\beta_1 \geq \dots \geq \beta_n$ , respectively, and let  $M = X - Y$ .
- **Weyl's theorem:**
  - $M$  is symmetric.
  - $|\alpha_i - \beta_i| \leq \|M\|$  for all  $i=1, \dots, n$ , where  $\|M\|$  is the largest eigenvalue of  $M$ .
- More generally:
  - Let  $v_1, \dots, v_n$  be an orthonormal basis of eigenvectors of  $A$  corresponding to  $\alpha_1, \dots, \alpha_n$  and let  $u_1, \dots, u_n$  be an orthonormal basis of eigenvectors of  $B$  corresponding to  $\beta_1, \dots, \beta_n$ . Let  $\theta_i$  be the angle between  $v_i$  and  $w_i$ . Then,

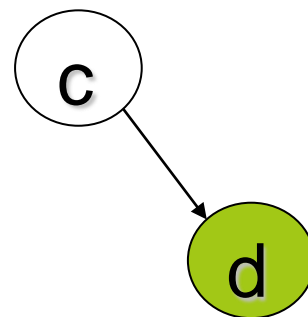
$$\frac{1}{2} \sin 2\theta_i \leq \frac{\|M\|}{\min_{j \neq i} |\alpha_i - \alpha_j|}$$

# Perturbation

- How robust is the spectrum under noise and minor structural perturbation?

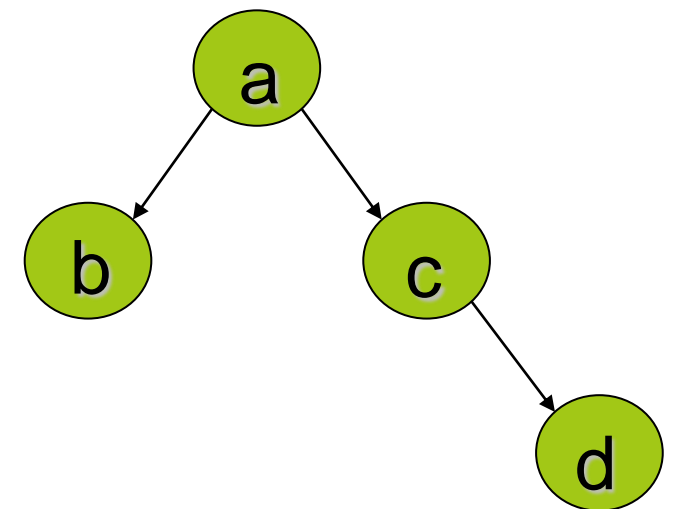


G (original)



E (noise)

=



H (perturbed)

	a	b	c	
a	0	1	1	0
b	-1	0	0	0
c	-1	0	0	0
	0	0	0	0

$\Psi(A_G)$

+

	a	b	c	d
a	0	0	0	0
b	0	0	0	0
c	0	0	0	1
d	0	0	-1	0

$A_E$

=

	a	b	c	
a	0	1	1	0
b	-1	0	0	0
c	-1	0	0	1
	0	0	-1	0

$A_H$

# Perturbation

- [Wilkinson] If  $A$  and  $A + E$  are  $n \times n$  symmetric matrices, then for all  $k$  in  $\{1, \dots, n\}$ , and eigenvalues  $\lambda_1 \geq \lambda_2 \geq \dots \geq \lambda_n$ :

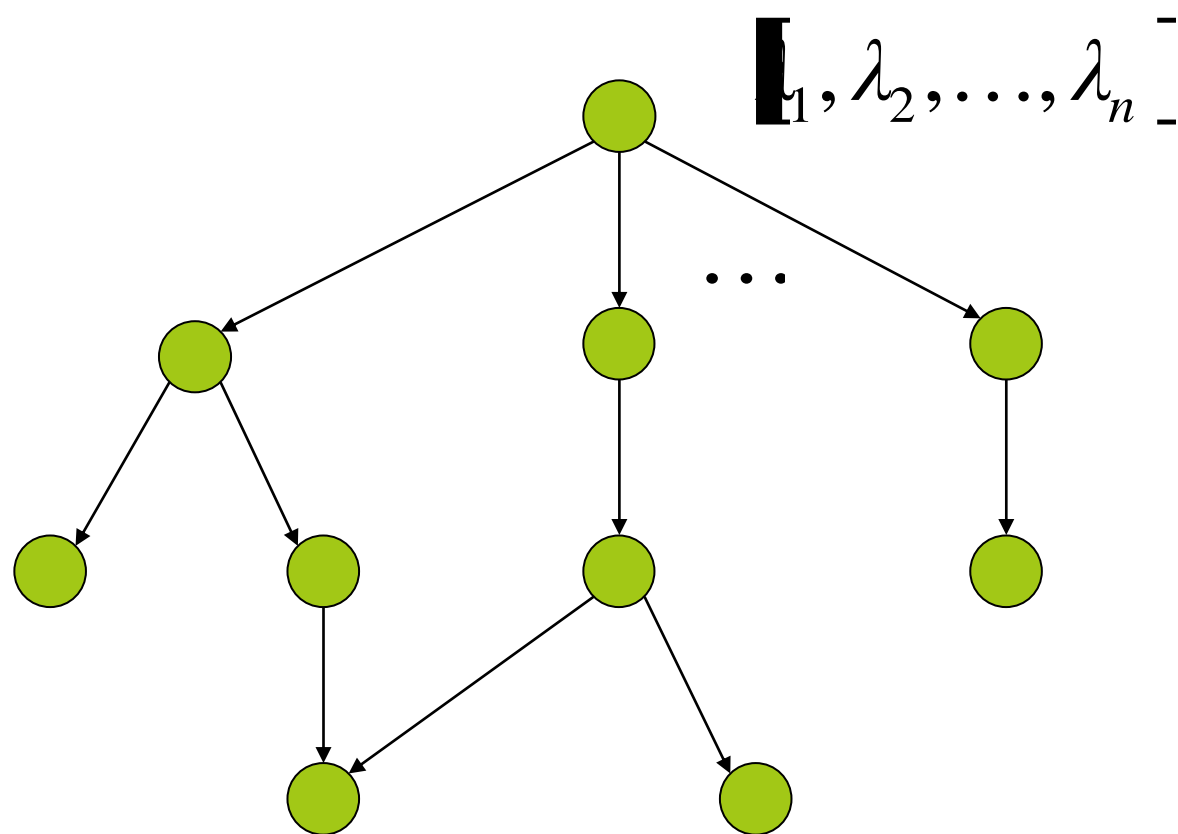
$$\lambda_k(A) + \lambda_k(E) \leq \lambda_k(A + E) \leq \lambda_k(A) + \lambda_1(E).$$

- This is also known as Courant's interlacing theorem
- [Marcini et al.] For  $H$  (perturbed graph) and  $G$  (original graph), the above theorem yields (after manipulation):

$$|\lambda_k(A_H) - \lambda_k(\Psi(A_G))| \leq |\lambda_1(A_E)|$$

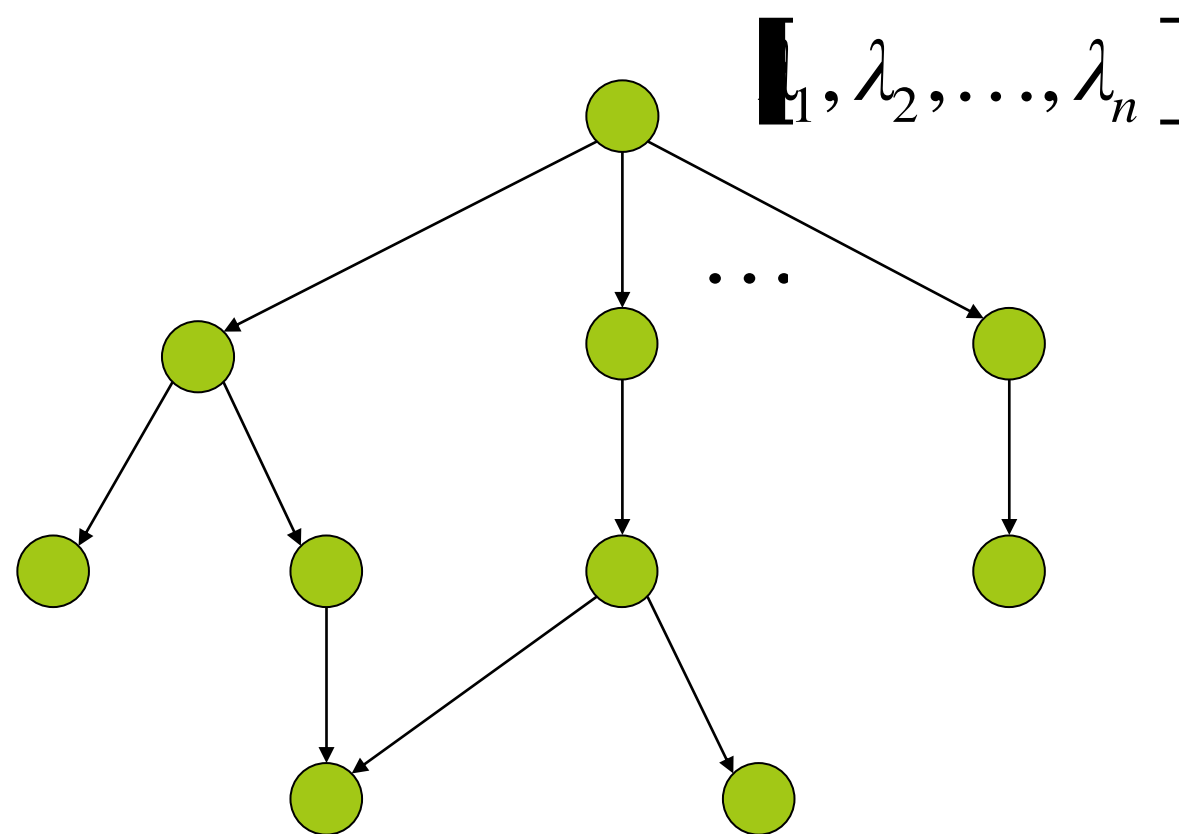
- They also extended this result to directed acyclic graphs.

# The Eigenvalues are Stable Now What?



We *could* compute the graph's eigenvalues, sort them, and let them become the components of a vector assigned to the graph.

# The Eigenvalues are Stable Now What?

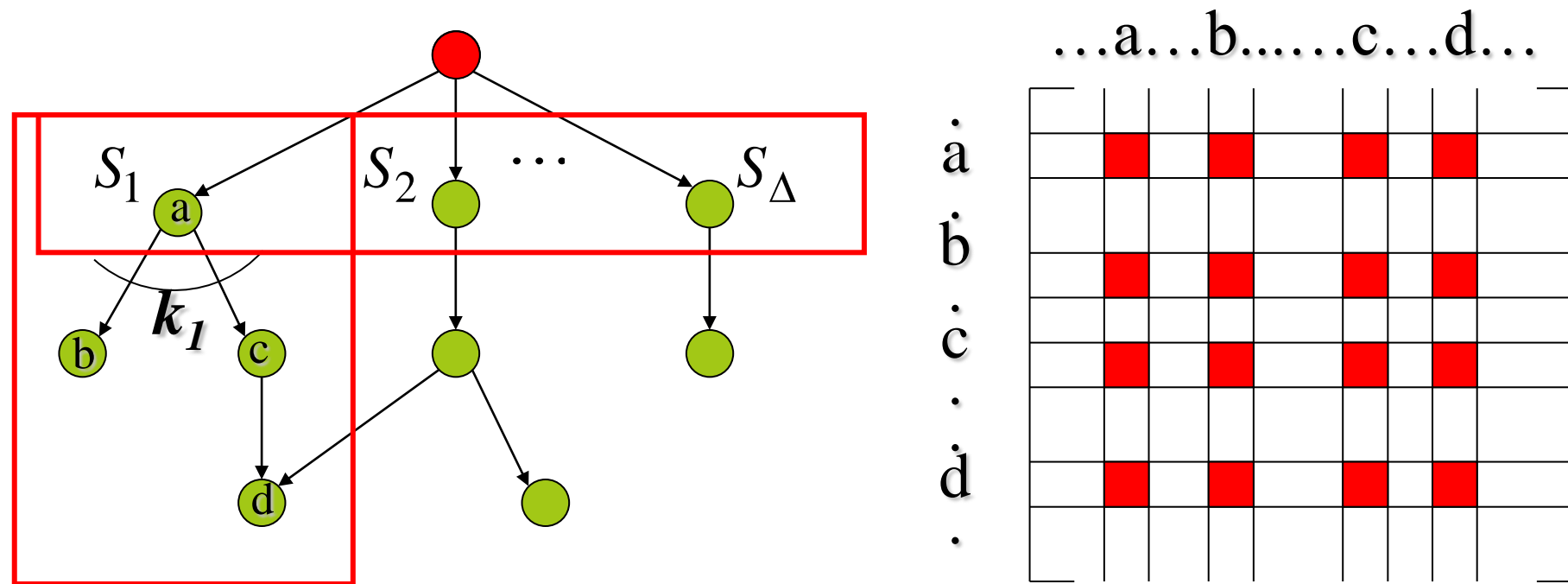


We *could* compute the graph's eigenvalues, sort them, and let them become the components of a vector assigned to the graph.

**But:**

1. Dimensionality grows with size of graph.
2. Eigenvalues are global! Therefore, can't accommodate occlusion or clutter.

# Forming a Structural Signature

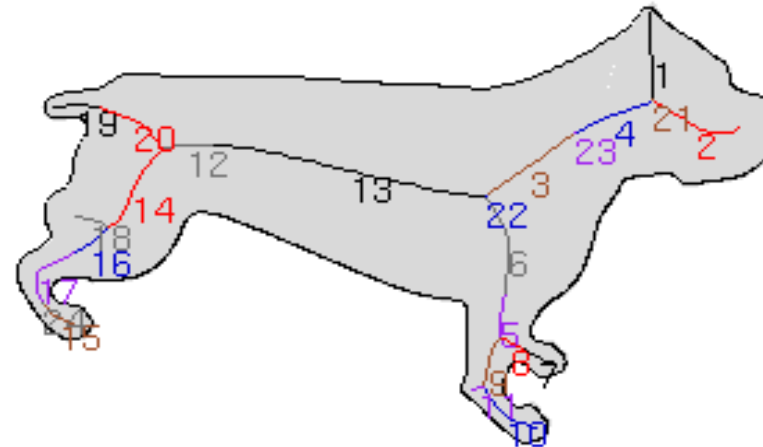
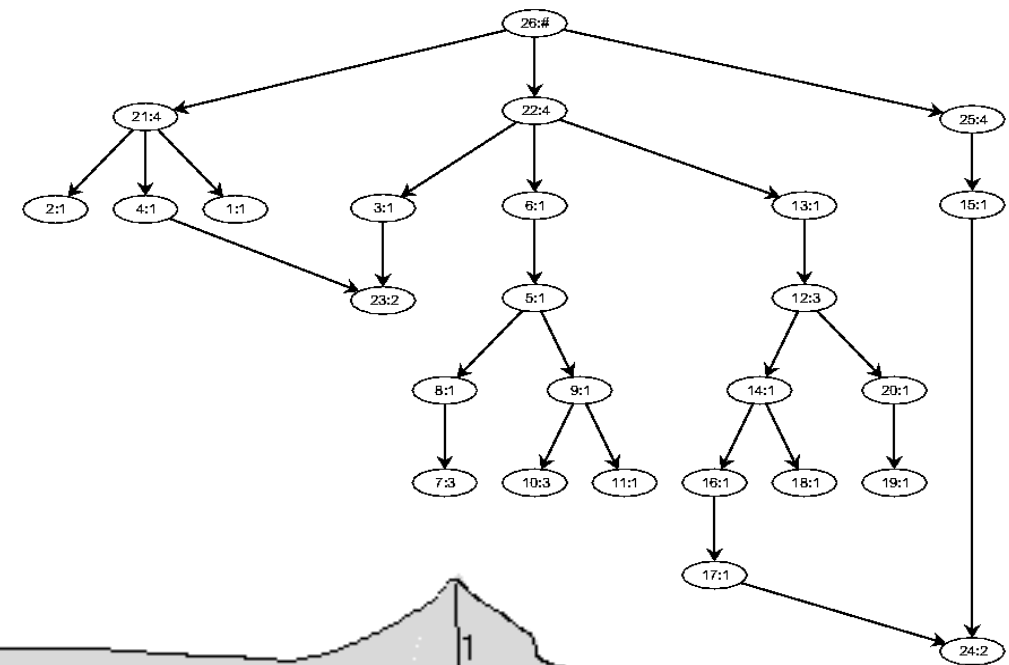
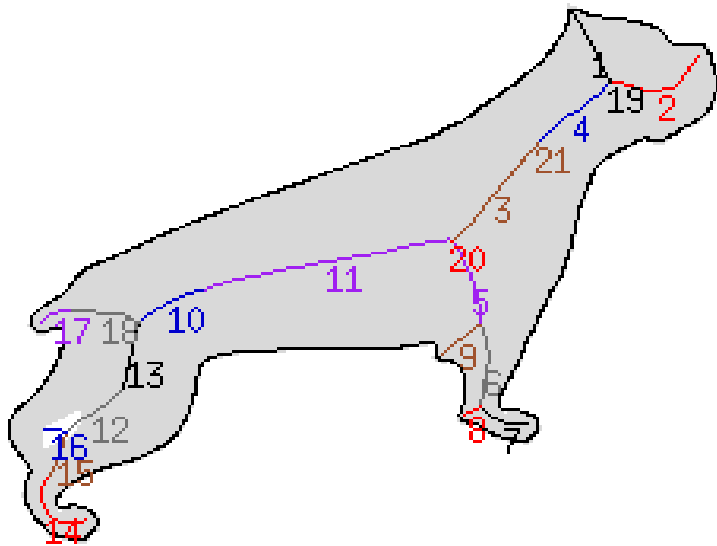
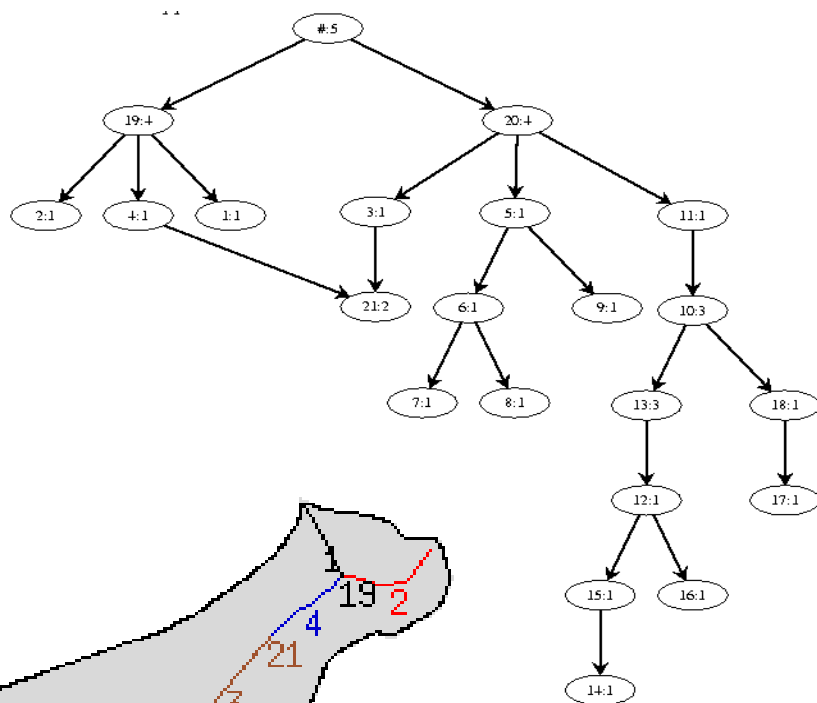


$$V = [S_1, S_2, S_3, \dots, S_\Delta], \quad S_1 \geq S_2 \geq S_3 \geq \dots S_\Delta \quad S_i = |\lambda_1| + |\lambda_2| + \dots |\lambda_{k_i}|$$

## Why Sum the $k$ largest Eigenvalues?

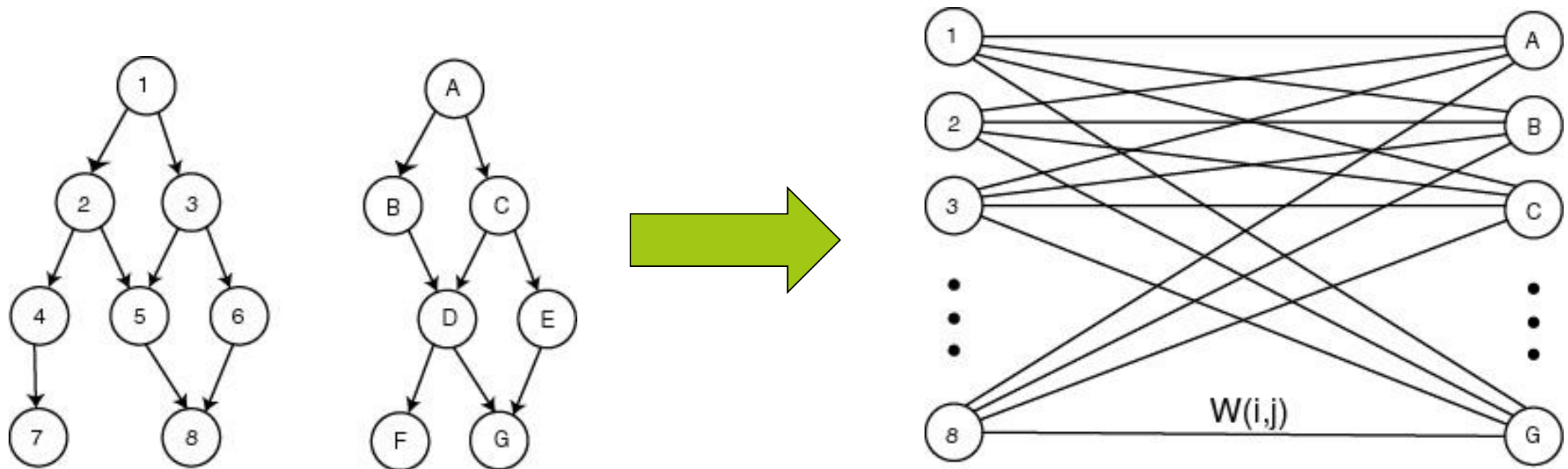
1. Summing reduces dimensionality.
2. Largest eigenvalues most informative.
3. Sums are “normalized” according to richness ( $k_i$ ) of branching structure.

# Matching Spectral Abstractions of Graph Structure





# Matching Problem:

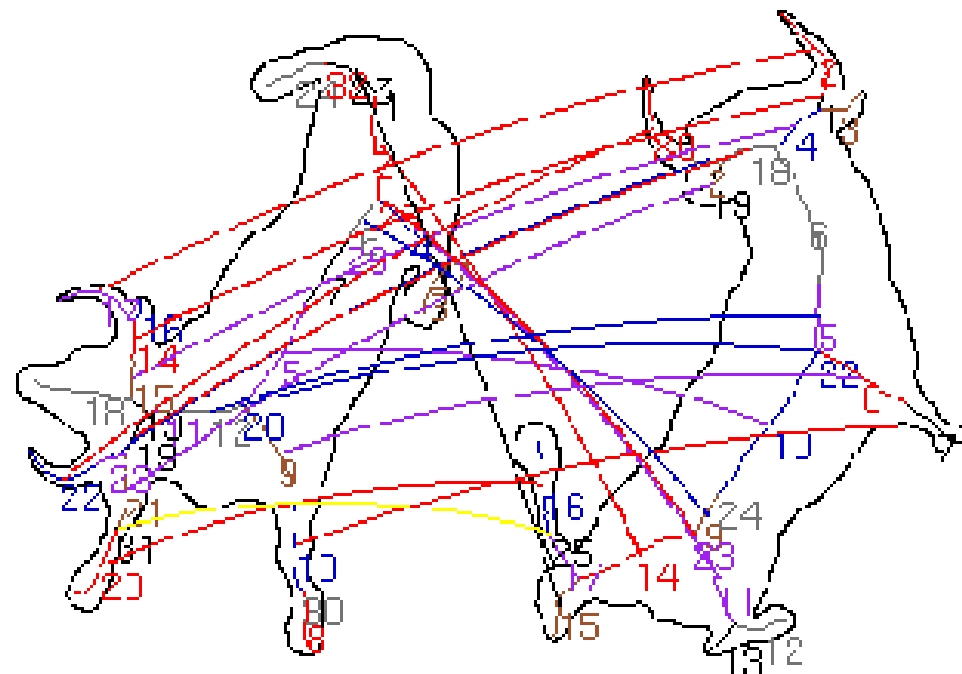
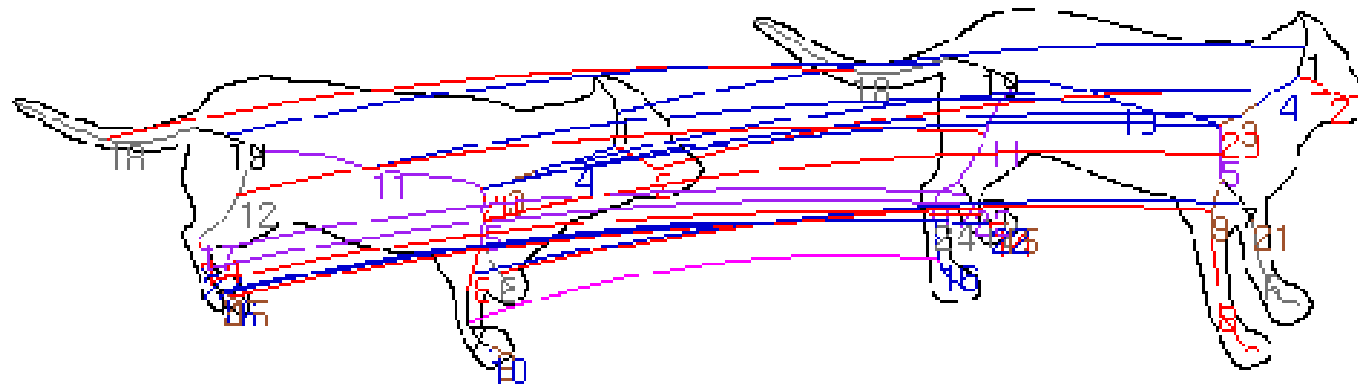


Matching: Consider a bipartite graph matching formulation, in which the edges in the query and model graphs are discarded.

Hierarchical structure is seemingly lost, but can be encoded in the edge weights:

$$W(i, j) = e^{-\alpha_1 d_{struct}(i, j) + \alpha_2 d_{geom}(i, j)}$$

# Sample Matches

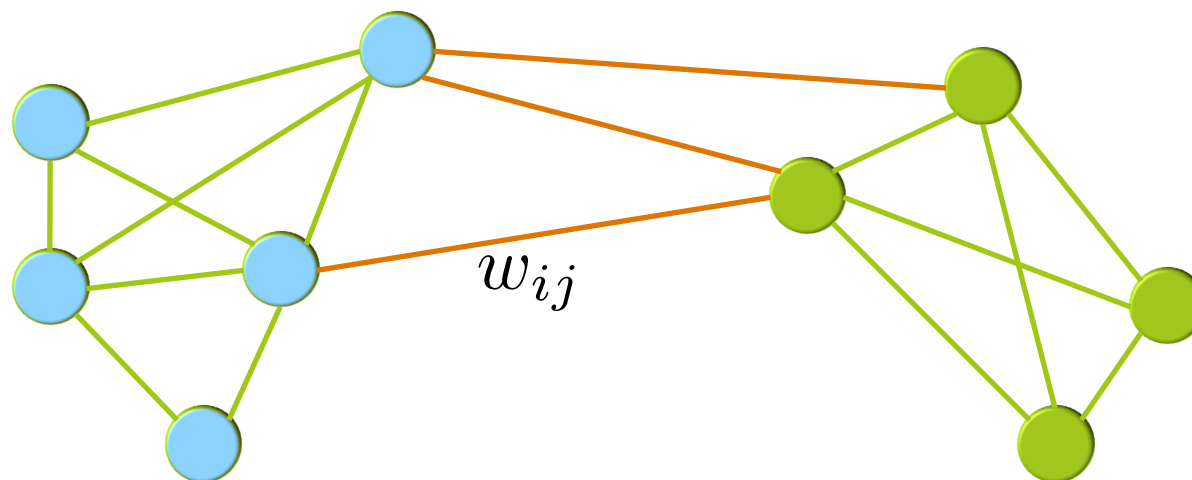


# Connectivity:

- Is there a relationship between eigenvalue distribution and structure of a graph?
- Not hard to show that  $\lambda_2(G) > 0$  iff  $G$  is connected.
- **Fiedler eigenvalue problem:** Better connected graphs have higher second eigenvalues!
- There is an eigen-embedding algorithm due to Fiedler (extended by Holst):
  - Compute the eigenvector  $\mathbf{x}_2$  corresponding to  $\lambda_2(G)$
  - Form a cut by  $S_{t(\leq 0)} = \{u \mid \mathbf{x}_2(u) > t\}$  (and  $V \setminus S_t$ )
  - Fiedler showed the set  $S_t$  forms a (strongly) connected subgraph.

# Cuts and Clustering:

- Recall a cut in a graph is a partition of the vertices to two sets  $S$ ,  $V-S$ .
- For a weighted graph a weight can be associated with the cut:



$$\mathbb{P}(S) = \text{cut}(S, V - S) = \sum_{i \in S} \sum_{j \in V-S} w_{ij}$$

# Connectivity and Graph Cut:

- Recall the tradeoff function for sparsest cut or min flux cut (ratio of cut) is:

$$R(S) = \frac{|E(S)|}{|S| \cdot |V - S|}.$$

- $R(S)$  is at least  $\lambda_2(G)/n$  and eigenvector  $v_2$  corresponding to second eigenvalue is related to indicator vector for a set  $S$  that minimizes  $R(S)$ :

# Connectivity and Graph Cut:

- Recall the tradeoff function for sparsest cut or min flux cut (ratio of cut) is:

$$R(S) = \frac{|\mathcal{E}(S)|}{|S| |V - S|}.$$

- $R(S)$  is at least  $\lambda_2(\mathbf{G})/n$  and eigenvector  $\mathbf{v}_2$  corresponding to second eigenvalue is related to indicator vector for a set  $S$  that minimizes  $R(S)$ :

- Let  $\mathbf{x}_S$  be the characteristic vector for  $S$ .

- We know  $\mathbf{x}_S^T \mathbf{L}_G \mathbf{x}_S = |\mathcal{E}(S)|$ .

- And  $\mathring{a}_{u < v}(\mathbf{x}_S(u) - \mathbf{x}_S(v))^2 = |S| |V - S|$ .

- So  $R(S) = \frac{\mathbf{x}_S^T \mathbf{L}_G \mathbf{x}_S}{\mathring{a}_{u < v}(\mathbf{x}_S(u) - \mathbf{x}_S(v))^2}$

# Connectivity and Partitioning:

- Recall the tradeoff function for sparse or min flux cut (ratio of cut) is:

$$R(S) = \frac{|\mathcal{E}(S)|}{|S| |V - S|}.$$

- $R(S)$  is at least  $\lambda_2(G)/n$  and eigenvector  $\mathbf{v}_2$  corresponding to second eigenvalue is related to indicator vector for a set  $S$  that minimizes  $R(S)$ :

- Let  $\mathbf{x}_S$  be the characteristic vector for  $S$ .

- We know  $\mathbf{x}_S^T L_G \mathbf{x}_S = |\mathcal{E}(S)|$ ,

- And  $\sum_{u < v} (\mathbf{x}_S(u) - \mathbf{x}_S(v))^2 = |S| |V - S|$ .

- So  $R(S) = \frac{\mathbf{x}_S^T L_G \mathbf{x}_S}{\sum_{u < v} (\mathbf{x}_S(u) - \mathbf{x}_S(v))^2}$

Fideler's eigenvalue problem

$$\lambda_2(G) = n^{-1} \min_{\mathbf{x} \neq 0} \frac{\mathbf{x}^T L_G \mathbf{x}}{\sum_{u < v} (\mathbf{x}(u) - \mathbf{x}(v))^2}$$

# Connectivity and Partitioning:

- Restricting the entries of vector  $\mathbf{x}$  being a 0-1 will result in the cut that minimizes  $R(S)$  and is the desirable min cut [**Hagen and Kahng**].

- The weighted variation of the  $R(S)$  can be stated as

$$F(S) = \frac{w(\P(S))}{d(S) d(V - S)}$$

- Which is proportional to normalized cut measure (Lawler and Sokal)

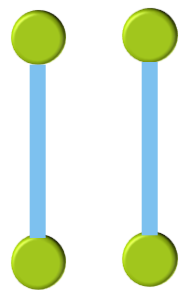
$$\frac{w(\P(S))}{d(S)} + \frac{w(\P(V - S))}{d(V - S)}$$

We will see that this is the objective function used by Shi and Malik for their segmentation algorithm.

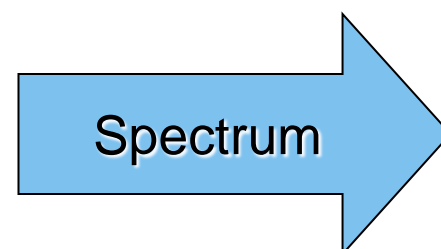


# Spectral Clustering

- Methods that use the spectrum of the affinity matrix to cluster are known as *spectral clustering*.
- Normalized cuts, Average cuts, Average association make use of the eigenvectors of the affinity matrix.



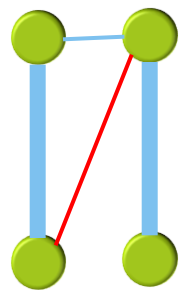
1	1	0	0
1	1	0	0
0	0	1	1
0	0	1	1



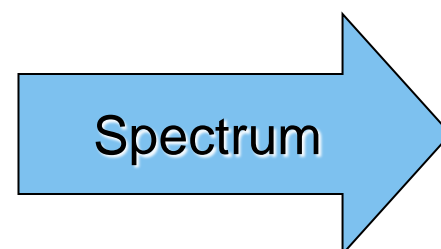
$\lambda_1=2$	$\lambda_2=2$	$\lambda_3=0$	$\lambda_4=0$
.71	0		
.71	0		
0	.71		
0	.71		

# Spectral Clustering

- Methods that use the spectrum of the affinity matrix to cluster are known as *spectral clustering*.
- Normalized cuts, Average cuts, Average association make use of the eigenvectors of the affinity matrix.



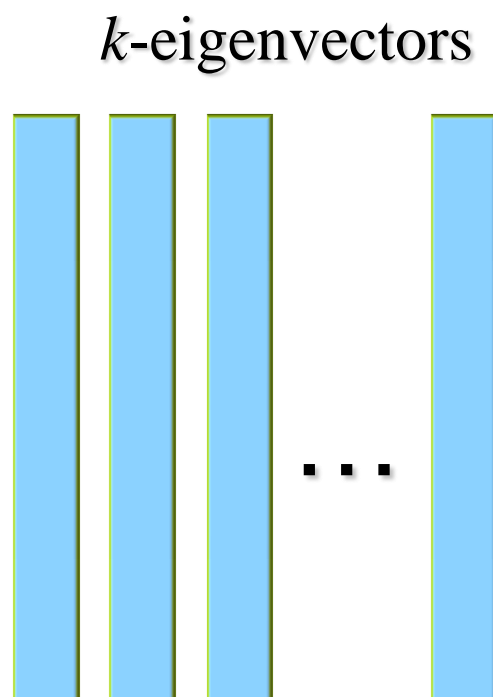
1	1	.2	0
1	1	0	-.2
.2	0	1	1
0	-.2	1	1



$\lambda_1 = 2.02$	$\lambda_2 = 2.02$	$\lambda_3 = -0.02$	$\lambda_4 = -0.02$
.71	0		
.69	-.14		
.14	.69		
0	.71		

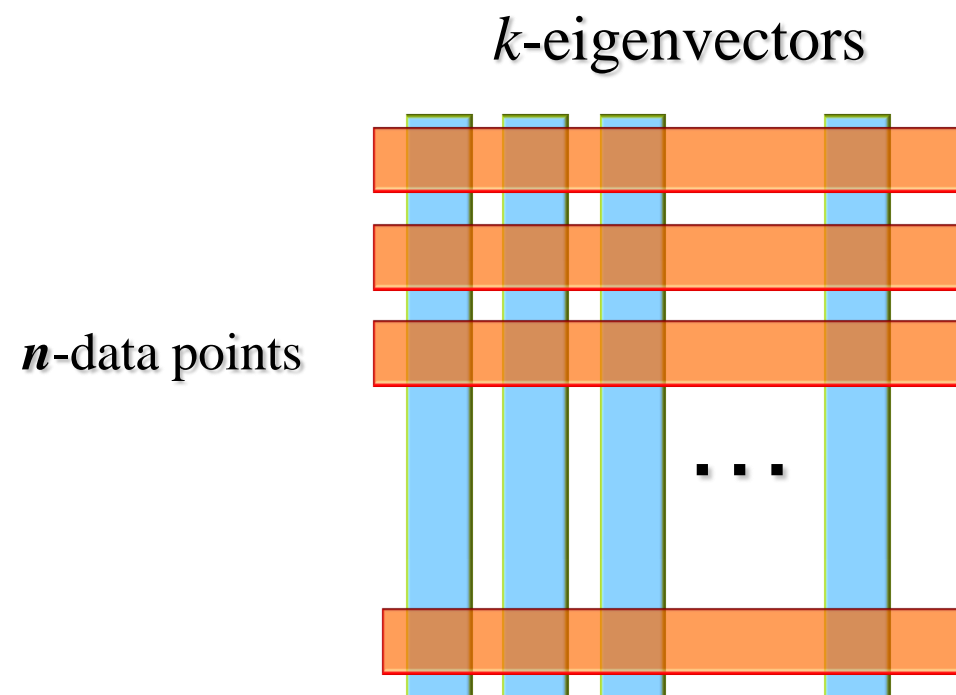
# Spectral Clustering

- We can use  $k$  eigenvectors for embedding of vertices into vector space.



# Spectral Clustering

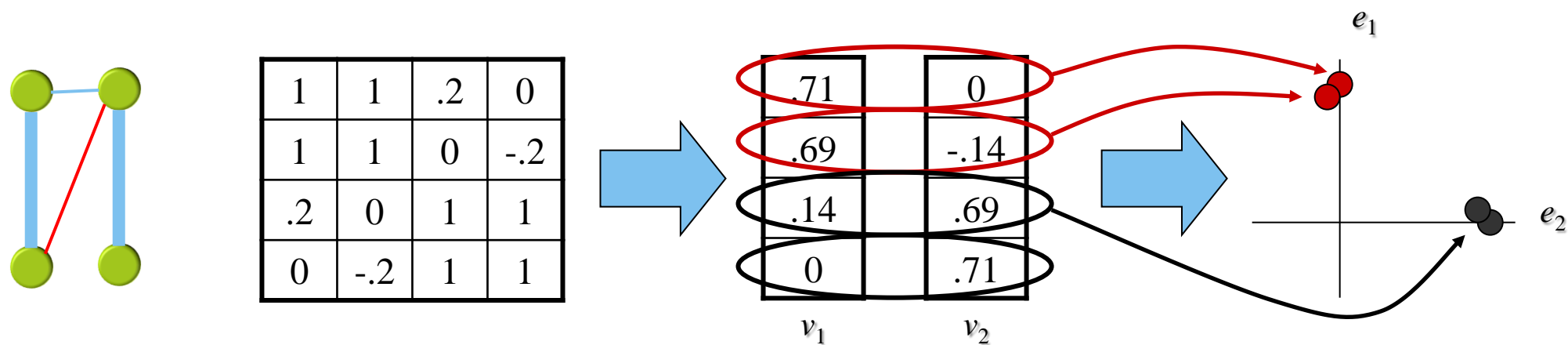
- We can use  $k$  eigenvectors for embedding of vertices into vector space.



- Each Row represents a data point in the eigenvector space.

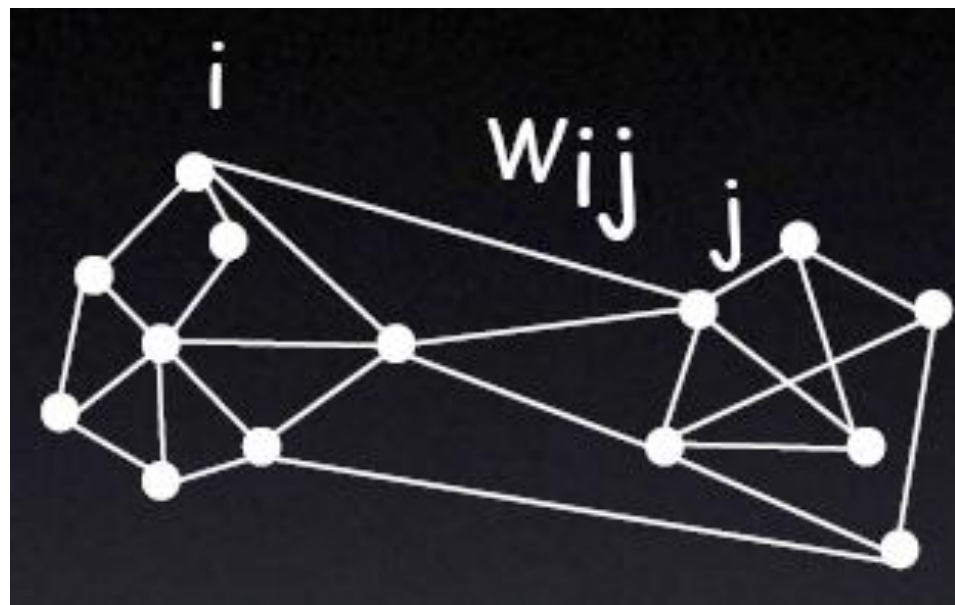
# Spectral Clustering

- We can use  $k$  eigenvectors for embedding of vertices into vector space.



- Each Row represents a data point in the eigenvector space.

# Graph-based Image Segmentation



$$G=(V,E)$$

$V$ : graph nodes



Pixels

$E$ : edges connection nodes



Pixel similarity

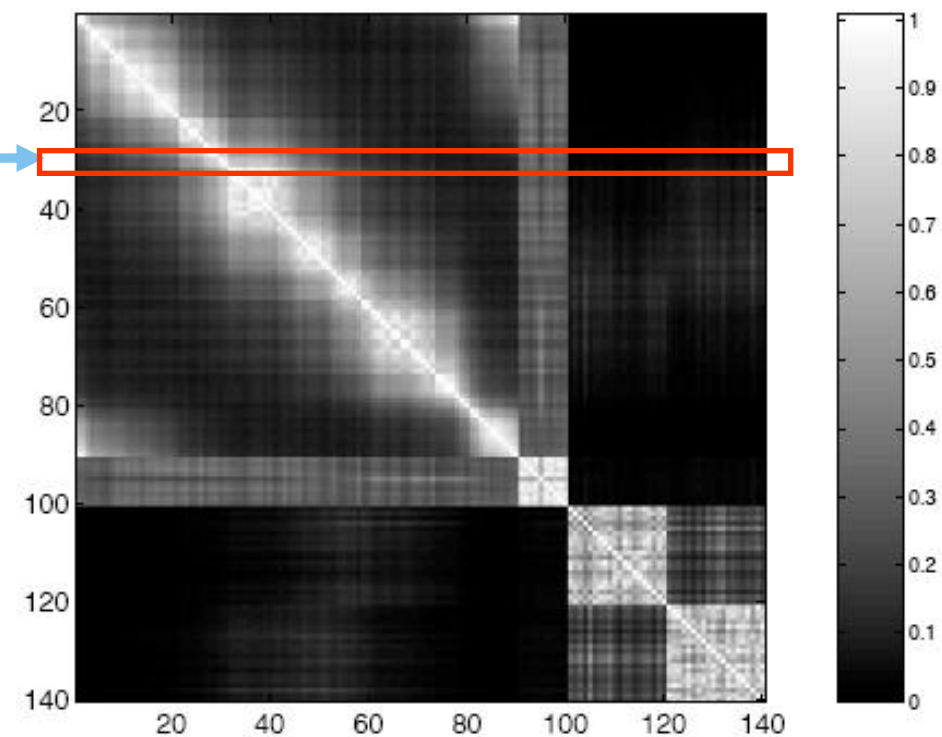
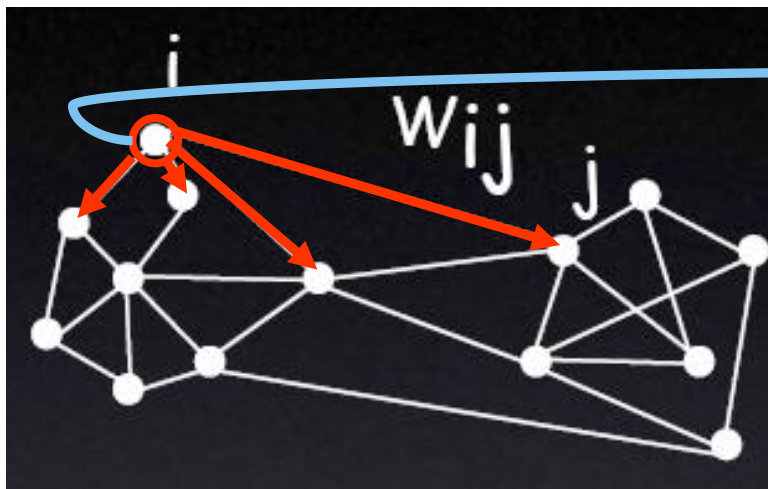
Slides from Jianbo Shi

# Cuts and segmentation

- Similarity matrix:

$$W = [w_{i,j}]$$

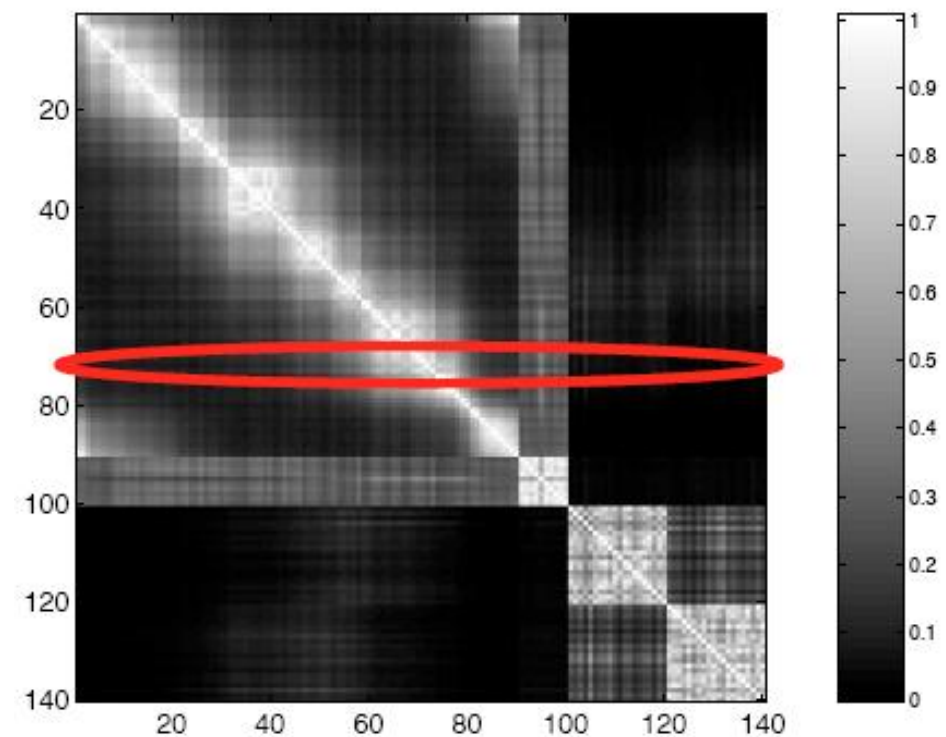
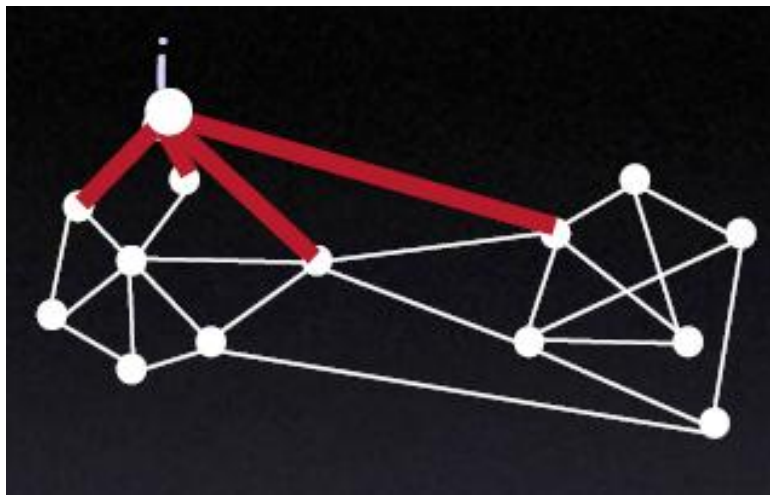
$$w_{i,j} = e^{\frac{-\|X_{(i)} - X_{(j)}\|_2^2}{s_X^2}}$$



# Graph terminology

□ Degree of node:

$$d_i = \sum_j w_{i,j}$$

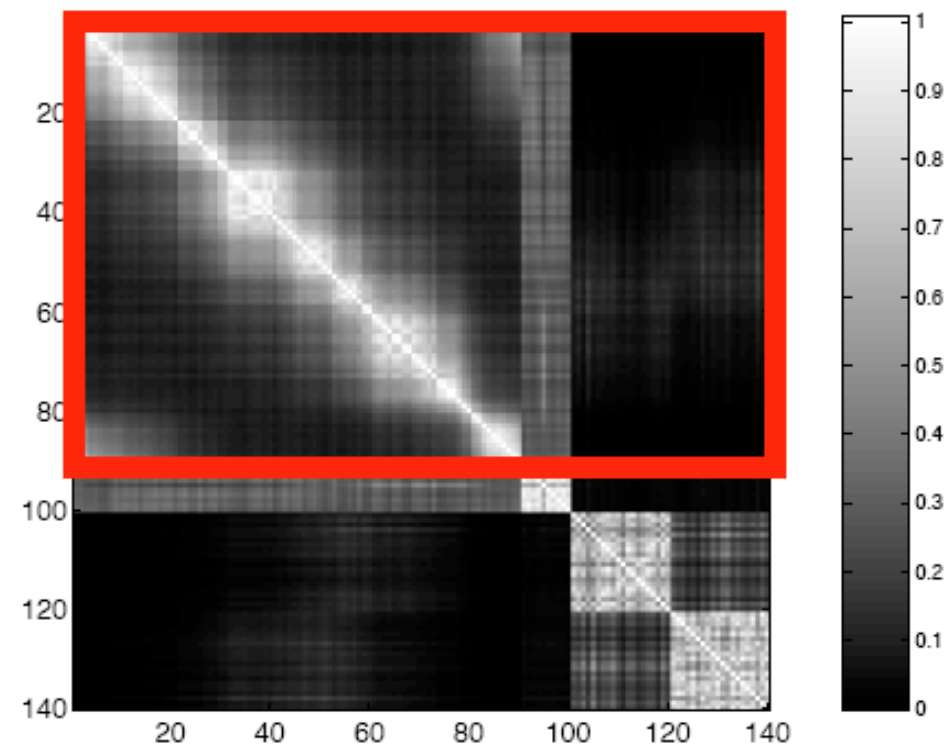
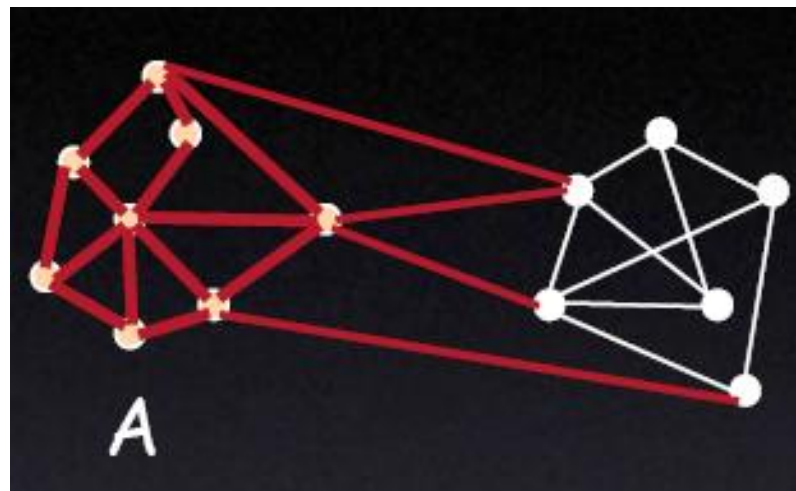




# Graph terminology

▣ Volume of set:

$$\text{vol}(A) = \text{assoc}(A, V) = \sum_{i \in A} d_i, A \subseteq V$$



Slides from Jianbo Shi

# Similarity functions

Intensity

$$W(i, j) = e^{\frac{-\|I_{(i)} - I_{(j)}\|_2^2}{\sigma_I^2}}$$

Distance

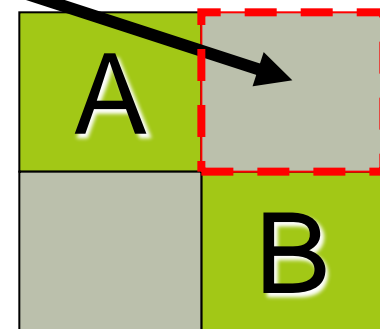
$$W(i, j) = e^{\frac{-\|X_{(i)} - X_{(j)}\|_2^2}{\sigma_X^2}}$$

Texture

$$W(i, j) = e^{\frac{-\|c_{(i)} - c_{(j)}\|_2^2}{\sigma_c^2}}$$

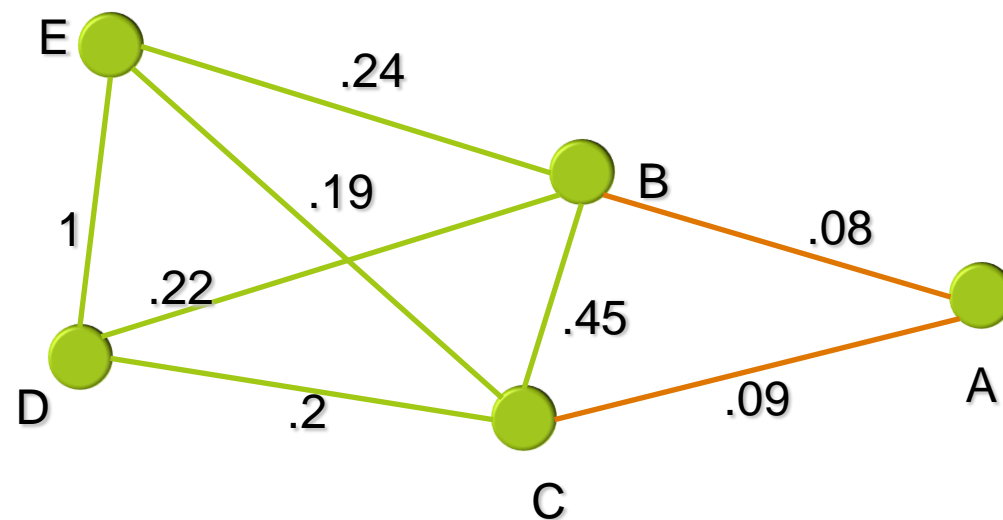
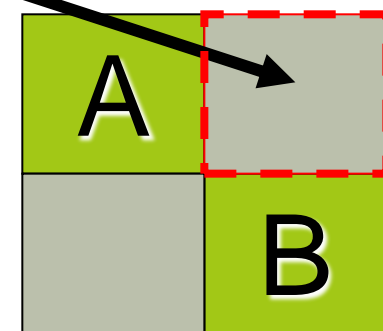
# Minimum cut

$$\min cut(A, B) = \min_{A, B} \sum_{u \in A, v \in B} w(u, v)$$



# Minimum cut

$$\min cut(A, B) = \min_{A, B} \sum_{u \in A, v \in B} w(u, v)$$

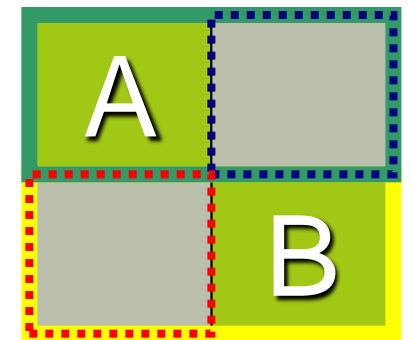


$$Cut(BCDE, A) = 0.17$$

# Normalized Cut

- Define normalized cut: “a fraction of the total edge connections to all the nodes in the graph”:

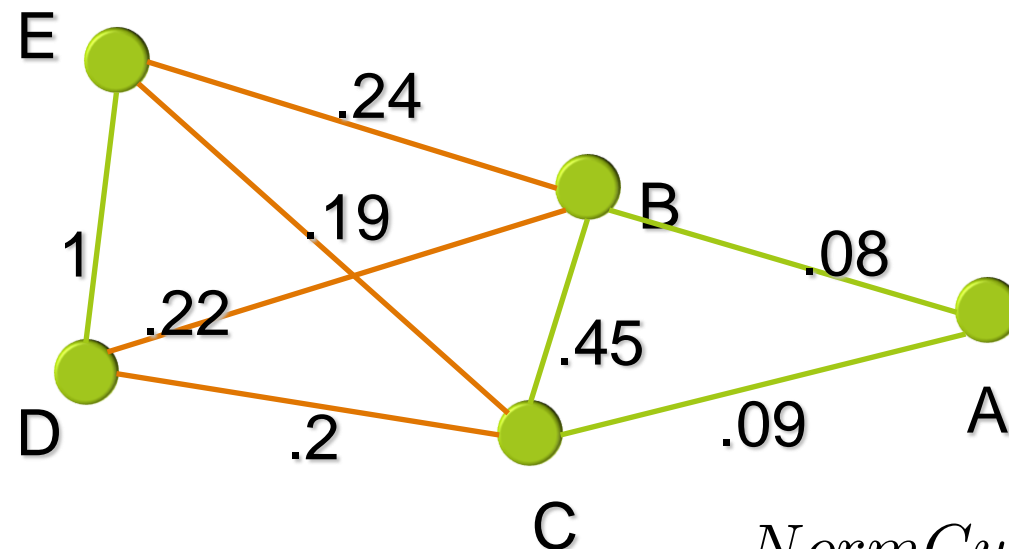
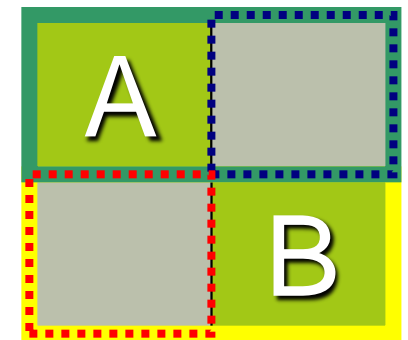
$$Ncut(A, B) = \frac{cut(A, B)}{assoc(A, V)} + \frac{cut(A, B)}{assoc(B, V)}$$



# Normalized Cut

- Define normalized cut: “a fraction of the total edge connections to all the nodes in the graph”:

$$Ncut(A, B) = \frac{cut(A, B)}{assoc(A, V)} + \frac{cut(A, B)}{assoc(B, V)}$$



$$NormCut(BCDE, A) = 1.067$$

$$NormCut(ABC, DE) = 1.038$$

# Finding the cut:

- Minimal (bi-partition) normalized cut.

$$\min \frac{Cut(C_1, C_2)}{Vol(C_1)} + \frac{Cut(C_1, C_2)}{Vol(C_2)} = \min \left( \frac{1}{Vol(C_1)} + \frac{1}{Vol(C_2)} \right) Cut(C_1, C_2)$$

# Finding the cut:

- Minimal (bi-partition) normalized cut.

$$\min \frac{Cut(C_1, C_2)}{Vol(C_1)} + \frac{Cut(C_1, C_2)}{Vol(C_2)} = \min \left( \frac{1}{Vol(C_1)} + \frac{1}{Vol(C_2)} \right) Cut(C_1, C_2)$$

- This can be restated in matrix form as

$$NCut(A, B) = \frac{y^T (D - W)y}{y^T D y}$$

- $D$  is the diagonal (weighted) degree matrix
- $W$  is the weighted adjacency matrix
- $D - W$  is the Laplacian matrix



# Finding the cut:

- Minimal (bi-partition) normalized cut.

$$\min \frac{Cut(C_1, C_2)}{Vol(C_1)} + \frac{Cut(C_1, C_2)}{Vol(C_2)} = \min \left( \frac{1}{Vol(C_1)} + \frac{1}{Vol(C_2)} \right) Cut(C_1, C_2)$$

- This can be restated in matrix form as

$$NCut(A, B) = \frac{y^T (D - W) y}{y^T D y}$$

- As an optimization problem:

$$\min_y y^T (D - W) y \text{ subject to } y^T D y = 1$$

# Finding the cut:

- Minimal (bi-partition) normalized cut.

$$\min \frac{Cut(C_1, C_2)}{Vol(C_1)} + \frac{Cut(C_1, C_2)}{Vol(C_2)} = \min \left( \frac{1}{Vol(C_1)} + \frac{1}{Vol(C_2)} \right) Cut(C_1, C_2)$$

- This can be restated in matrix form as

$$NCut(A, B) = \frac{y^T (D - W)y}{y^T D y}$$

- As an optimization problem:

$$\min_y y^T (D - W)y \text{ subject to } y^T D y = 1$$

- Which is a generalized eigenvalue problem:

$$(D - W)y = \lambda D y$$

# Recall

- $L = D - W$  Positive semi-definite  $x^T L x \geq 0$

- The first eigenvalue is 0, eigenvector is  $\vec{1}$

- The second eigenvalue contains the solution

$$\lambda_2 = \frac{Cut(A, B)}{|A|} + \frac{Cut(A, B)}{|B|}$$

- The corresponding eigenvector contains the cluster indicator for each data point

# Random walks:

- Recall  $W_G$  denotes the normalized Laplacian of  $G$ .
- Let  $\omega_1 \geq \dots \geq \omega_n$  the spectrum of  $W_G$ ; where  $\omega_1$  is equal to 1 and has multiplicity 1. Let  $d$  denote eigenvector corresponding to  $\omega_1$ . We can define a probability distribution vector  $\pi$  for graph  $G$  as follows:

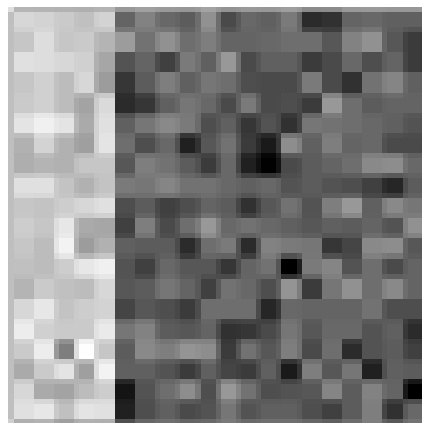
$$p(G) = \frac{1}{\sum_u d(u)} d$$

- If  $\omega_n \neq -1$ , then the distribution of every walk will converge to  $\pi$ .
- The rate of converge is a function of  $|\omega_1 - \max(|\omega_2|, |\omega_n|)|$ .
- Specifically, let  $x_t(v)$  denote the state of the system after  $t$  steps for a walk starting at  $u$ :

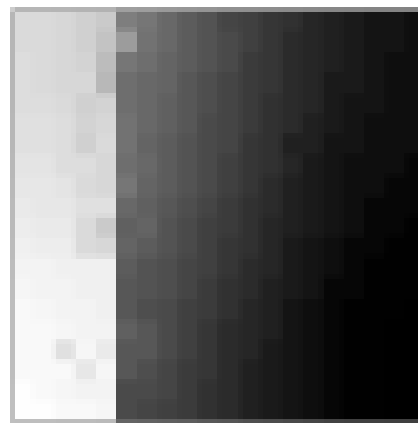
$$|p_t(b) - p(b)| \leq \sqrt{\frac{d(v)}{d(u)}} \left(1 - \max(|\omega_2|, |\omega_n|)\right)$$

# Experiments

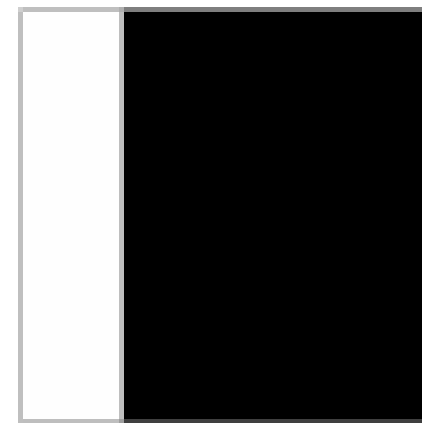
## ■ Synthetic images:



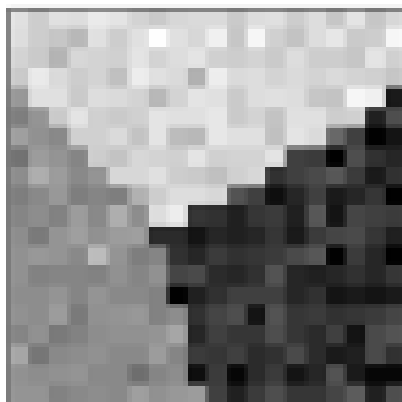
(a)



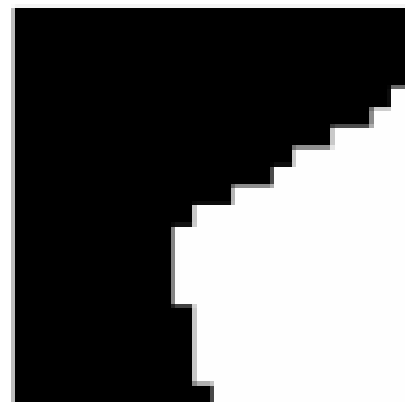
(b)



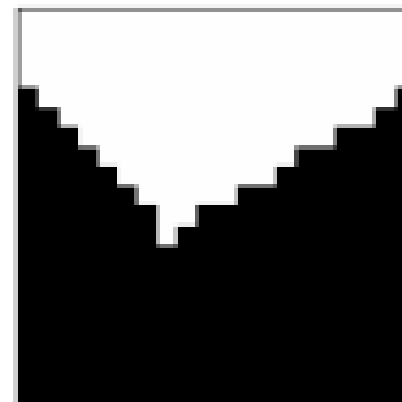
(c)



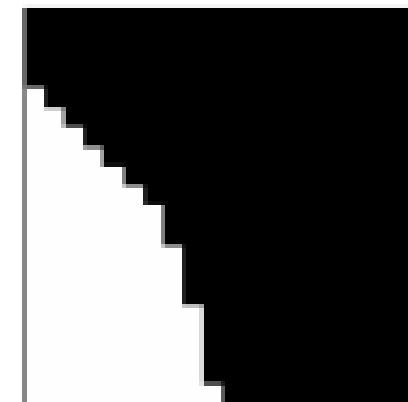
(a)



(b)



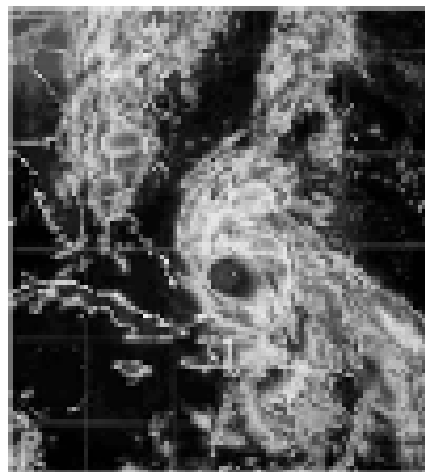
(c)



(d)

# Experiments

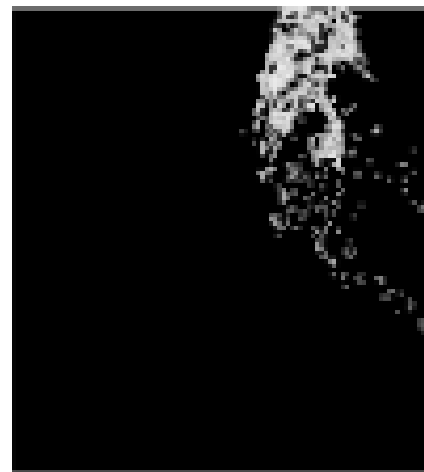
## Weather radar:



(a)



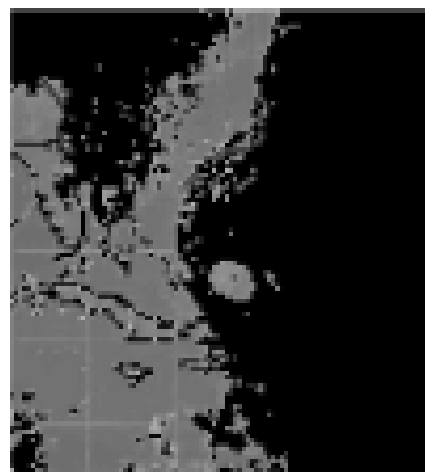
(b)



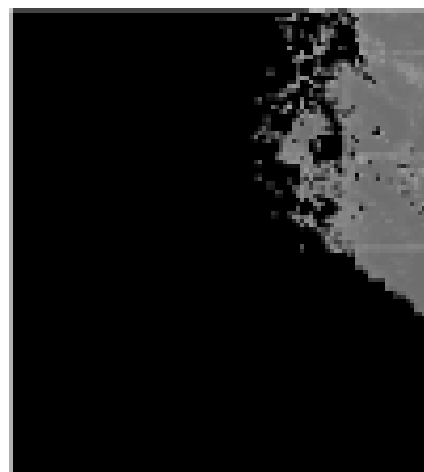
(c)



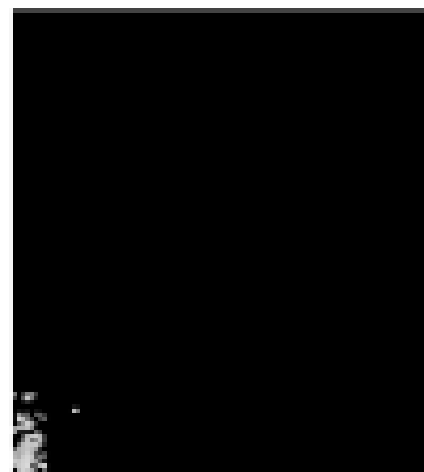
(d)



(e)



(f)



(g)

# Experiments



(a)



(b)



(c)



(d)



(e)



(f)



(g)

# Coloring:

- Valid coloring:
  - Given a graph  $G$ , assign a color to every vertex of  $G$  so that the endpoints of each edge receive distinct colors.
- As an optimization the objective is to use minimum number of colors.
- The chromatic number  $\chi(G)$  is the least  $k$  for which  $G$  has a valid  $k$ -coloring.
- [Wilf] Let  $\alpha_1 \geq \dots \geq \alpha_n$  denote the spectrum of graph then

$$\chi(G) \leq 1 + \alpha_1$$

- [Hoffman] If  $G$  is a graph with at least one edge, then

$$\chi(G) \leq 1 + \frac{\alpha_1}{-\alpha_n}$$



# Independent Sets:

- An independent set of vertices of graph  $G$ , is a subset of vertices  $S$  such that no edge has both its end points in  $S$ .
- As an optimization the objective is to find a maximum size independent set, denoted by  $\rho(G)$ .
- Note that the vertices of any color class of a graph  $G$  form an independent set:

$$\rho(G) \geq \frac{n}{c(G)}$$

- [Hoffman] If  $G$  is a degree  $d$  regular graph, then

$$\rho(G) \leq n \cdot \frac{d - a_n}{d}$$

# References

- Doyle, P. G. and Snell, J. L., Random Walks and Electric Networks, Vol. 22 of Carus Mathematical Monographs, Mathematical Association of America, 1984.
- Chung, F. R. K., Spectral Graph Theory, American Mathematical Society, 1997.
- van der Holst, H., Lov`asz, L., and Schrijver, A., “The Colin de Verdi`ere Graph Parameter,” Bolyai Soc. Math. Stud., Vol. 7, 1999, pp. 29–85.
- Cvetkovi´c, D. M., Doob, M., and Sachs, H., Spectra of Graphs, Academic Press, 1978.
- Fiedler, M., “Algebraic connectivity of graphs,” Czechoslovak Mathematical Journal , Vol. 23, No. 98, 1973, pp. 298–305.
- Fiedler, M., “A property of eigenvectors of nonnegative symmetric matrices and its applications to graph theory,” Czechoslovak Mathematical Journal , Vol. 25, No. 100, 1975, pp. 618–633.

# References

- Lovász, L., "Random walks on graphs: a survey," Combinatorics, Paul Erdős is Eighty, Vol. 2, edited by T. S. D. Miklos, V. T. Sos, Janos Bolyai Mathematical Society, Budapest, 1996, pp. 353–398.
- Wilf, H. S., "The Eigenvalues of a Graph and its Chromatic Number," J. London math. Soc., Vol. 42, 1967, pp. 330–332.
- Hoffman, A. J., "On eigenvalues and colorings of graphs," Graph Theory and its Applications, Academic Press, New York, 1970, pp. 79–92.
- Dodziuk, J., "Difference Equations, Isoperimetric Inequality and Transience of Certain Random Walks," Transactions of the American Mathematical Society, Vol. 284, No. 2, 1984, pp. 787–794.
- Pothen, A., Simon, H. D., and Liou, K.-P., "Partitioning Sparse Matrices with Eigenvectors of Graphs," SIAM Journal on Matrix Analysis and Applications, Vol. 11, No. 3, 1990, pp. 430–452.