Community Detection: Spectral Clustering

CS224W: Analysis of Networks
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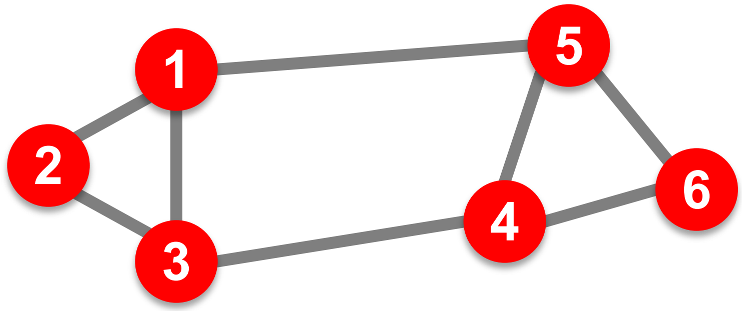
http://cs224w.stanford.edu

Spectral Clustering Algorithms

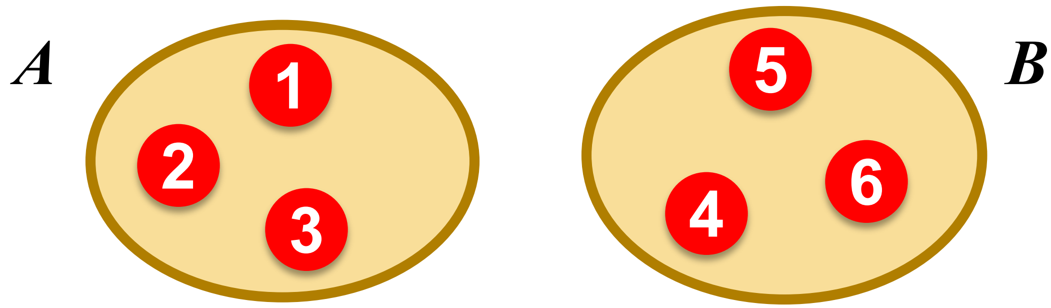
- **Three basic stages:**
  - **1) Pre-processing**
    - Construct a matrix representation of the graph
  - **2) Decomposition**
    - Compute eigenvalues and eigenvectors of the matrix
    - Map each point to a lower-dimensional representation based on one or more eigenvectors
  - **3) Grouping**
    - Assign points to two or more clusters, based on the new representation
- But first, let's define the problem

Graph Partitioning

- **Undirected graph $G(V, E)$:**



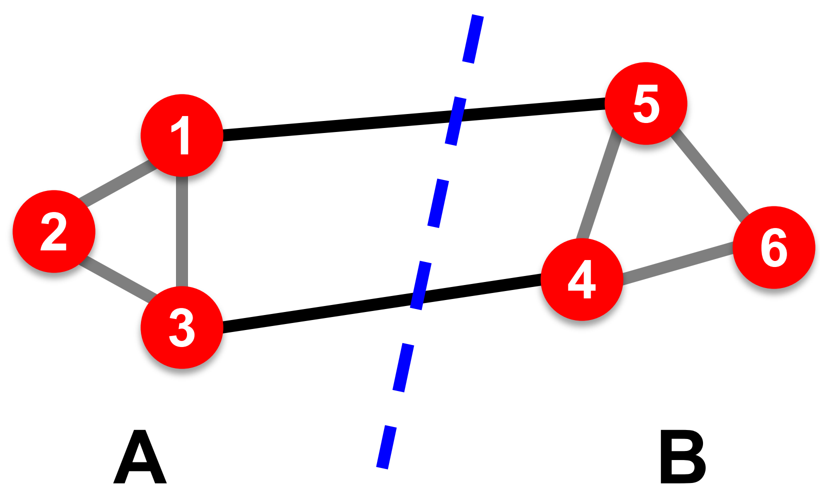
- **Bi-partitioning task:**
  - Divide vertices into two disjoint groups A, B



- **Questions:**
  - How can we define a “good” partition of G?
  - How can we efficiently identify such a partition?

Graph Partitioning

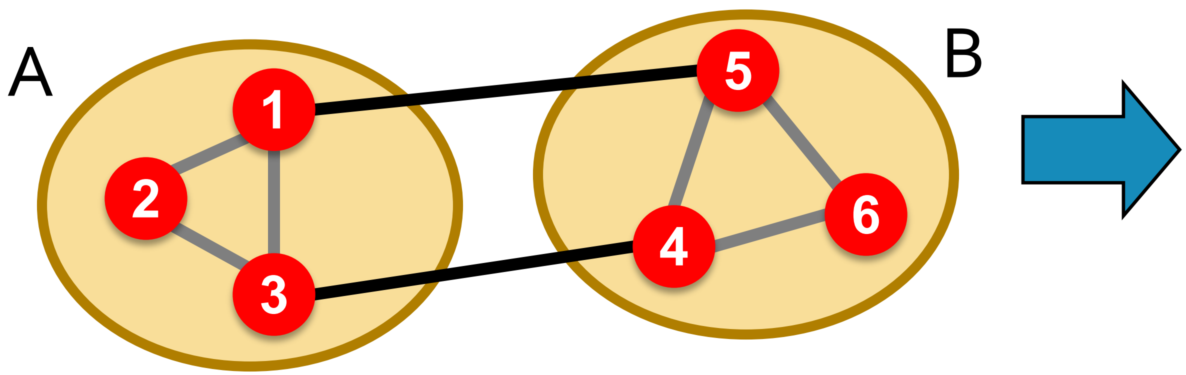
- **What makes a good partition?**
  - Maximize the number of within-group connections
  - Minimize the number of between-group connections



Graph Cuts

- **Express partitioning objectives as a function of the “edge cut” of the partition**
- **Cut:** Set of edges with only one vertex in a group: $$cut(A,B) = \sum_{i\in A, j\in B} w_{ij}$$

If the graph is weighted w_{ij} is the weight, otherwise, all w_{ij}={0,1}



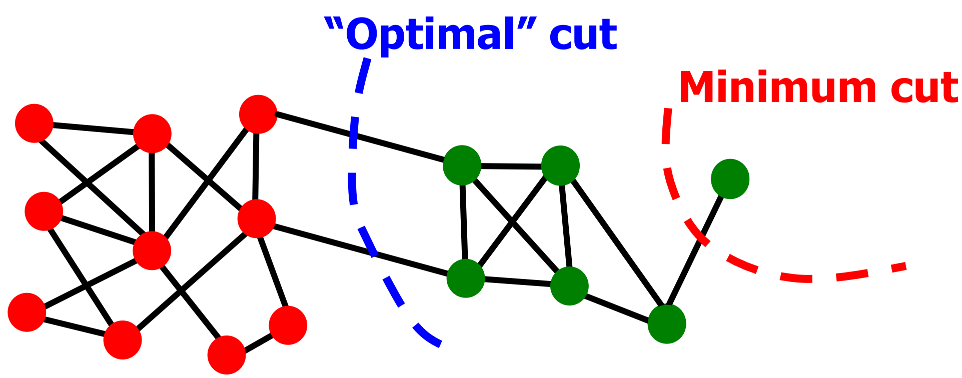
$cut(A,B) = 2$

Graph Cut Criterion

- **Criterion: Minimum-cut**
  - Minimize weight of connections between groups

$$\arg\min_{A,B} \mathit{cut}(A,B)$$

- **Degenerate case:**



- **Problem:**
  - Only considers external cluster connections
  - Does not consider internal cluster connectivity

Graph Cut Criterion

- **Criterion: Conductance** [Shi-Malik, '97]
  - Connectivity between groups relative to the density of each group

$$\phi(A,B) = \frac{cut(A,B)}{\min(vol(A), vol(B))}$$

$\boldsymbol{vol(A)}$: total weighted degree of the nodes in $\boldsymbol{A}$: $\boldsymbol{vol(A) = \sum_{i \in A} k_i}$ (number of edge end points in $\boldsymbol{A}$)

- **Why use this criterion?**
  - Produces more balanced partitions
- **How do we efficiently find a good partition?**
  - **Problem:** Computing best conductance cut is NP-hard

Spectral Graph Partitioning

- A: adjacency matrix of undirected **G**
  - A_{ij} **=1** if $(\boldsymbol{i}, \boldsymbol{j})$ is an edge, else **0**
- $\boldsymbol{x}$ is a vector in $\Re^n$ with components $(\boldsymbol{x_1}, \dots, \boldsymbol{x_n})$
  - Think of it as a label/value of each node of $\boldsymbol{G}$
- **What is the meaning of $A \cdot x$?**

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} y_1 \\ \vdots \\ y_n \end{bmatrix}$$

$$y_i = \sum_{j=1}^{n} A_{ij} x_j = \sum_{(i,j) \in E} x_j$$

- **Entry y_i is a sum of labels x_j of neighbors of i**

What is the meaning of *Ax*?

- j^{th} **coordinate of $A \cdot x$:**
  - Sum of the x-values of neighbors of j
  - Make this a new x-value at node j

$$\begin{bmatrix} a_{11} & \dots & a_{1n} \\ \vdots & & \vdots \\ a_{n1} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \lambda \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix}$$

$$\boldsymbol{A \cdot x = \lambda \cdot x}$$

- **Spectral Graph Theory:**
  - Analyze the "spectrum" of matrix representing $\boldsymbol{G}$
  - **Spectrum:** Eigenvectors $\boldsymbol{x}^{(i)}$ of a graph, ordered by the magnitude (strength) of their corresponding eigenvalues $\boldsymbol{\lambda_i}$: $\quad \Lambda = \{\lambda_1, \lambda_2, \dots, \lambda_n\}$

$$\lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$$

Note: We sort λ_i in ascending (not descending) order!

Example: d-regular graph

- Suppose all nodes in $\boldsymbol{G}$ have degree $\boldsymbol{d}$ ($\boldsymbol{G}$ is $\boldsymbol{d}$-regular) and $\boldsymbol{G}$ is connected
- **What are some eigenvalues/vectors of $\boldsymbol{G}$?**

  $\boldsymbol{A} \cdot \boldsymbol{x} = \boldsymbol{\lambda} \cdot \boldsymbol{x}$ What is $\boldsymbol{\lambda}$? What $\boldsymbol{x}$?

  - **Let's try:** $\boldsymbol{x} = (\mathbf{1}, \mathbf{1}, \dots, \mathbf{1})$
  - **Then:** $\boldsymbol{A} \cdot \boldsymbol{x} = (\boldsymbol{d}, \boldsymbol{d}, \dots, \boldsymbol{d}) = \boldsymbol{\lambda} \cdot \boldsymbol{x}$. **So:** $\boldsymbol{\lambda} = \boldsymbol{d}$
  - **We found an eigenpair of $\boldsymbol{G}$:** $\boldsymbol{x} = (\mathbf{1}, \mathbf{1}, \dots, \mathbf{1}), \boldsymbol{\lambda} = \boldsymbol{d}$
- $\boldsymbol{d}$ is the largest eigenvalue of $\boldsymbol{A}$ (see next slide)

Remember the meaning of $\boldsymbol{y} = \boldsymbol{A} \cdot \boldsymbol{x}$:

$$y_i = \sum_{j=1}^{n} A_{ij} x_j = \sum_{(i,j) \in E} x_j$$

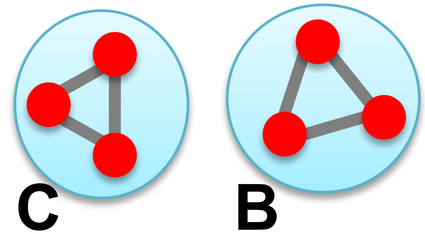
Note, this is just one eigenpair. An *n* by *n* matrix can have up to *n* eigenpairs.

d is the largest eigenvalue of A

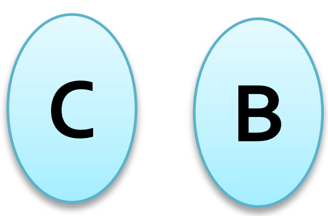
Details!

- $\boldsymbol{G}$ is $\boldsymbol{d}$-regular connected, $\boldsymbol{A}$ is its adjacency matrix
- **Claim:**
  - (1) $\boldsymbol{d}$ has multiplicity of **1** (there is only **1** eigenvector associated with eigenvalue $\boldsymbol{d}$)
  - (2) **d** is the largest eigenvalue of $\boldsymbol{A}$
- **Proof:**
  - To obtain value eigval $\boldsymbol{d}$ we needed $\boldsymbol{x_i} = \boldsymbol{x_j}$ for every i, j
  - This means $\boldsymbol{x} = c \cdot (1,1, \dots, 1)$ for some const. c
  - **Define:** Set $\boldsymbol{S}$ = nodes $\boldsymbol{i}$ with maximum value of $\boldsymbol{x_i}$
  - Then consider some vector $\boldsymbol{y}$ which is not a multiple of vector $(\mathbf{1}, \dots, \mathbf{1})$. So not all nodes $\boldsymbol{i}$ (with labels $\boldsymbol{y_i}$) are in $\boldsymbol{S}$
  - Consider some node $\boldsymbol{j} \in \boldsymbol{S}$ and a neighbor $\boldsymbol{i} \notin \boldsymbol{S}$ then node $\boldsymbol{j}$ gets a value strictly less than $\boldsymbol{d}$
  - So y is not eigenvector! And so $\boldsymbol{d}$ is the largest eigenvalue!

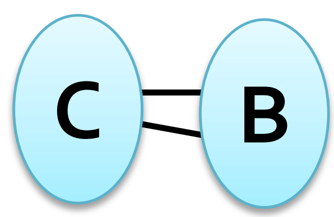
Example: Graph on 2 components



- **What if G is not connected?**
  - G has **2** components, each d-regular
- **What are some eigenvectors?**
  - $x =$ Put all 1s on C and 0s on B or vice versa
    - $x' = (\underbrace{1,\dots,1}_{|C|},\underbrace{0,\dots,0}_{|B|})^T$ **then** $\mathbf{A}\cdot x' = (d,\dots,d,0,\dots,0)^T$
    - $x'' = (0,\dots,0,1,\dots,1)^T$ **then** $A\cdot x'' = (0,\dots,0,d,\dots,d)^T$
    - And so in both cases the corresponding $\lambda = d$
- **A bit of intuition:**



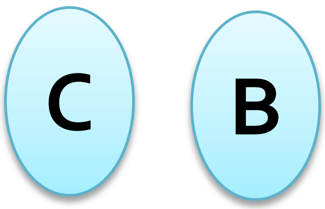
$\lambda_n = \lambda_{n-1}$



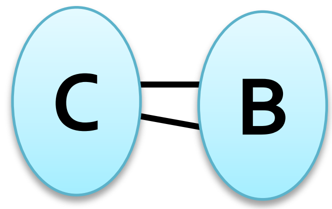
$\lambda_n - \lambda_{n-1} \approx 0$

2nd largest eigval. λ_{n-1} now has value very close to λ_n

More Intuition



$\lambda_n = \lambda_{n-1}$



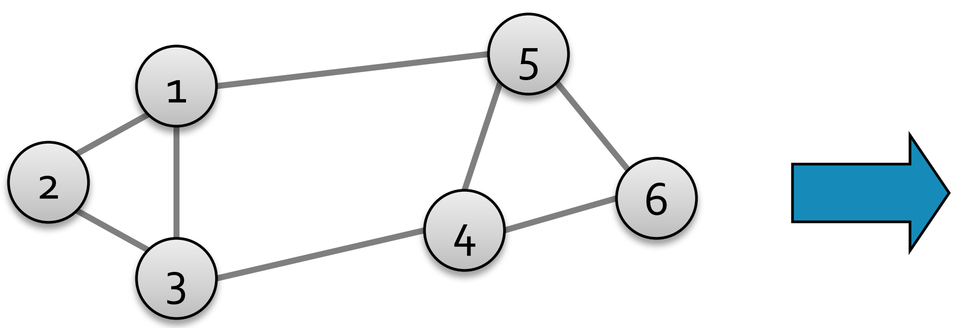
$\lambda_n - \lambda_{n-1} \approx 0$

2nd largest eigval. λ_{n-1} now has value very close to λ_n

- If the graph is connected (right example) then we already know that $\boldsymbol{x_n} = (\mathbf{1}, \dots \mathbf{1})$ is an eigenvector
- Eigenvectors are orthogonal so then the components of $\boldsymbol{x_{n-1}}$ must sum to **0**
  - Why? $\boldsymbol{x_n} \cdot \boldsymbol{x_{n-1}} = \mathbf{0}$ then $\sum_i \boldsymbol{x_n}[\boldsymbol{i}] \cdot \boldsymbol{x_{n-1}}[\boldsymbol{i}]$ = $\sum_i \boldsymbol{x_n}\ [\boldsymbol{i}]$
  - $\boldsymbol{x_{n-1}}$ "splits" the nodes into two groups
    - $\boldsymbol{x_{n-1}}[\boldsymbol{i}] > \mathbf{0}$ vs. $\boldsymbol{x_{n-1}}[\boldsymbol{i}] < \mathbf{0}$
  - So we in principle could look at the eigenvector of the 2nd largest eigenvalue and declare nodes with positive label in **C** and negative label in **B.** (but there are still many details for us to figure out here)

Matrix Representations

- **Adjacency matrix (A):**
  - $n \times n$ matrix
  - $A=[a_{ij}]$, $a_{ij}=1$ if edge between node i and j

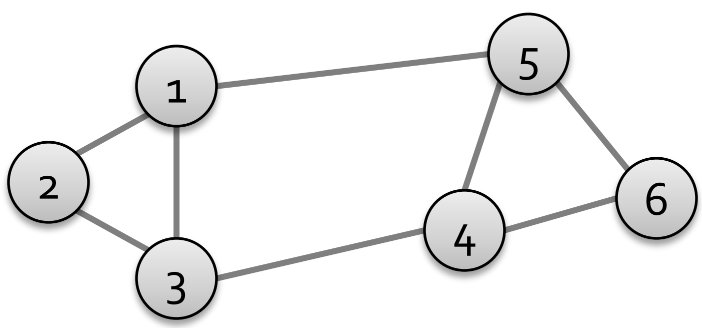


	1	2	3	4	5	6
1	0	1	1	0	1	0
2	1	0	1	0	0	0
3	1	1	0	1	0	0
4	0	0	1	0	1	1
5	1	0	0	1	0	1
6	0	0	0	1	1	0

- **Important properties:**
  - **Symmetric matrix**
  - **Has n real eigenvalues**
  - **Eigenvectors are real-valued and orthogonal**

Matrix Representations

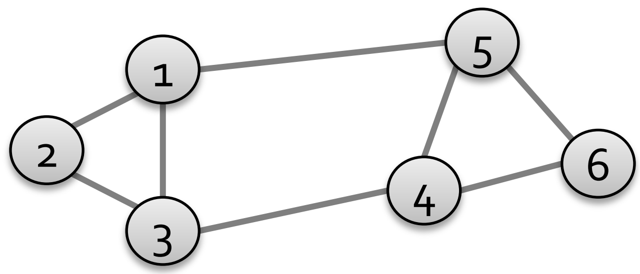
- **Degree matrix (D):**
  - $n \times n$ diagonal matrix
  - $D=[d_{ii}]$, d_{ii} = degree of node i



	1	2	3	4	5	6
1	3	0	0	0	0	0
2	0	2	0	0	0	0
3	0	0	3	0	0	0
4	0	0	0	3	0	0
5	0	0	0	0	3	0
6	0	0	0	0	0	2

Matrix Representations

- **Laplacian matrix (L):**
  - $n \times n$ symmetric matrix



	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

$$\boxed{L = D - A}$$

- **What is trivial eigenpair?**
  - $x = (1, \dots, 1)$ then $L \cdot x = 0$ and so $\lambda = \lambda_1 = 0$
- **Important properties of L:**
  - **Eigenvalues** are non-negative real numbers
  - **Eigenvectors** are real (and always orthogonal)

3 Facts about the Laplacian *L*

Details!

(a) All eigenvalues are ≥ 0

(b) $x^T L x = \sum_{ij} L_{ij} x_i x_j \geq 0$ for every x

(c) $L = N^T \cdot N$

- That is, L is positive semi-definite

- **Proof: (the 3 facts are saying the same thing)**
  - **(c)⇒(b):** $x^T L x = x^T N^T N x = (xN)^T (Nx) \geq 0$
    - As it is just the square of length of Nx
  - **(b)⇒(a):** Let $\boldsymbol{\lambda}$ be an eigenvalue of $\boldsymbol{L}$. Then by **(b)** $x^T L x \geq 0$ so $x^T L x = x^T \lambda x = \lambda x^T x \Rightarrow \boldsymbol{\lambda \geq 0}$
  - **(a)⇒(c):** is also easy! Do it yourself.

λ_2 as optimization problem

See next slide for the proof. Deriving this is a HW problem.

- **Fact: For symmetric matrix M:**

$$\lambda_2 = \min_{x \,:\, x^T w_1 = 0} \frac{x^T M x}{x^T x}$$

($\mathbf{w_1}$ is eigenvector corresponding to λ_1)

- **What is the meaning of min $x^{\mathrm{T}} L\, x$ on G?**
  - $x^T L\, x = \sum_{i,j=1}^{n} L_{ij}\, x_i x_j = \sum_{i,j=1}^{n} \left(D_{ij} - A_{ij}\right) x_i x_j$
  - $= \sum_i D_{ii} x_i^2 - \sum_{(i,j)\in E} 2 x_i x_j$
  - $= \sum_{(i,j)\in E} (\underbrace{x_i^2 + x_j^2} - 2 x_i x_j) = \boldsymbol{\sum_{(i,j)\in E} \left(x_i - x_j\right)^2}$

Node $\boldsymbol{i}$ has degree $\boldsymbol{d_i}$. So, value $\boldsymbol{x_i^2}$ needs to be summed up $\boldsymbol{d_i}$ times.
But each edge $(\boldsymbol{i}, \boldsymbol{j})$ has two endpoints so we need $\boldsymbol{x_i^2} + \boldsymbol{x_j^2}$

Details!

Proof: $\lambda_2 = \min_{x \,:\, x^T w_1 = 0} \frac{x^T M x}{x^T x}$

- Write x in basis of eigenvecs $w_1, w_2, \dots, w_n$ of $\boldsymbol{M}$. So, $x = \sum_i^n \alpha_i w_i$
- Then we get: $Mx = \sum_i \alpha_i \underbrace{M w_i}_{\boldsymbol{\lambda_i w_i}} = \sum_i \alpha_i \lambda_i w_i$
- So, what is $\boldsymbol{x^T M x}$?
  - $x^T M x = \overbrace{\left(\sum_i \alpha_i w_i\right)^T}^{\boldsymbol{x^T}} \overbrace{\left(\sum_i \alpha_i \lambda_i w_i\right)}^{\boldsymbol{Mx}} = \sum_{ij} \alpha_i \lambda_j \alpha_j \overbrace{w_i^T w_j}^{= 0 \text{ if } i \neq j,\ 1 \text{ otherwise}}$
    $= \sum_i \alpha_i^2 \lambda_i w_i^T w_i = \boldsymbol{\sum_i \lambda_i \alpha_i^2}$
  - Want minimize this over all unit vectors $\boldsymbol{w}$:
    $\boldsymbol{w}$ = min over choices of $(\alpha_1, \dots \alpha_n)$ so that:
    where $\sum \alpha_i^2 = 1$ (unit length) $\sum \alpha_i = 0$ (orthogonal to $\boldsymbol{w_1}$)
  - To minimize this, set $\boldsymbol{\alpha_2 = 1}$ and so $\boldsymbol{\sum_i \lambda_i \alpha_i^2 = \lambda_2}$

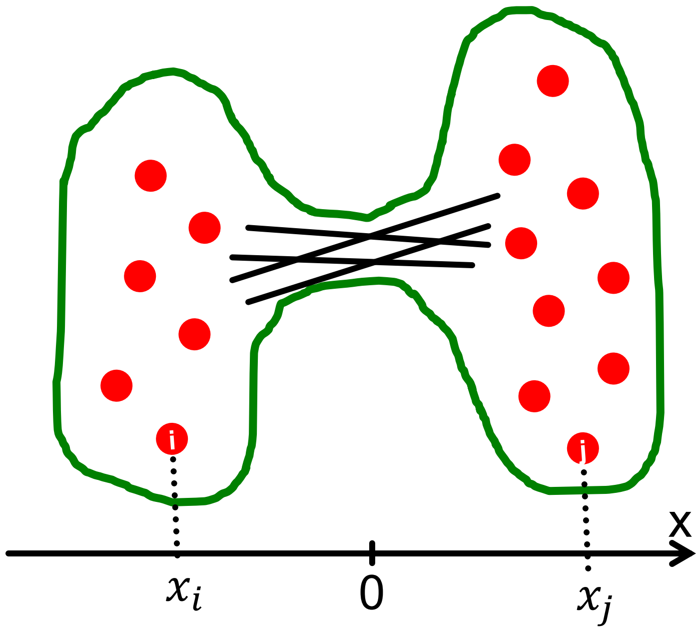
Finding x

$$\lambda_2 = \min_{x \,:\, x^T w_1 = 0} \frac{x^T M x}{x^T x}$$

- **What else do we know about x?**
  - x is unit vector: $\sum_i x_i^2 = 1$
  - x is orthogonal to 1st eigenvector $(1, \dots, 1)$ thus: $\sum_i x_i \cdot 1 = \sum_i x_i = 0$
- **Remember:**

$$\lambda_2 = \min_{\substack{\text{All labelings} \\ \text{of nodes } i \text{ so} \\ \text{that } \sum x_i = 0}} \frac{\sum_{(i,j)\in E} (x_i - x_j)^2}{\sum_i x_i^2}$$

We want to assign values x_i to nodes i such that few edges cross 0.
(we want x_i and x_j to subtract each other)



Balance to minimize

Find Optimal Cut [Fiedler'73]

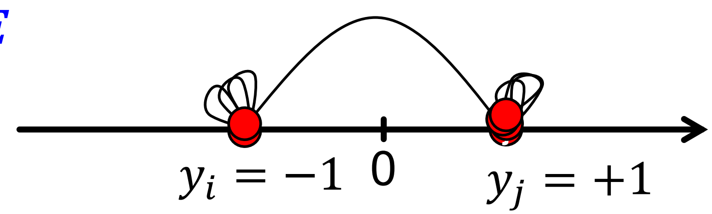
- **Back to finding the optimal cut**
- **Express partition (A,B) as a vector**

$$y_i = \begin{cases} +1 & if\ i \in A \\ -1 & if\ i \in B \end{cases}$$

- Enforce that $|A| = |B| \rightarrow \Sigma_i y_i = 0$
  - Equivalent to being orthogonal to the trivial eigenvector $(1, \dots, 1)$
- We can minimize the cut of the partition by finding a vector y that **minimizes**:

$$\arg \min_{y \in \{-1,+1\}^n} f(y) = \sum_{(i,j) \in E} (y_i - y_j)^2$$

Can't solve exactly. Let's relax y and allow it to take any real value.

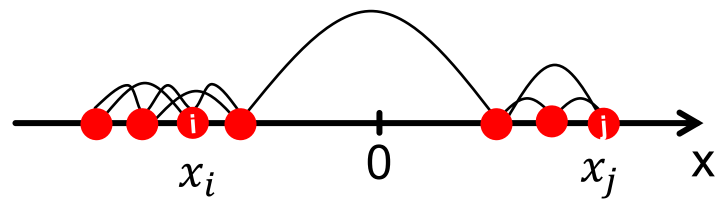


Rayleigh Theorem

$$\lambda_2 = \min_{x\,:\,x^T w_1 = 0} \frac{x^T M x}{x^T x}$$

Slide 18

$$\min_{\substack{y \in \mathbb{R}^n\,:\,\sum_i y_i = 0 \\ \sum_i y_i^2 = 1}} f(y) = \sum_{(i,j)\in E} (y_i - y_j)^2 = y^T L y$$



- $\boldsymbol{\lambda_2 = \min_y f(y)}$: The minimum value of $f(y)$ is given by the 2nd smallest eigenvalue λ_2 of the Laplacian matrix L
- $\mathbf{x = \arg\min_y} \boldsymbol{f(y)}$: The optimal solution for y is given by the corresponding eigenvector x, referred to as the **Fiedler vector**
- Can use sign of x_i to determine cluster assignment of node i

Approx. Guarantee of Spectral

Details!

- Suppose there is a partition of **G** into **A** and **B** where $|A| \leq |B|$, s.t. "conductance" of the cut (A,B) is $\boldsymbol{\alpha} = \frac{(\#\, edges\ from\ A\ to\ B)}{|A|}$ then $\boldsymbol{\lambda_2} \leq 2\boldsymbol{\alpha}$

  Note: |A|<|B|

  - This is the approximation guarantee of the spectral clustering: Spectral finds a cut that has at most **twice the conductance** as the optimal one of conductance $\boldsymbol{\alpha}$.
- **Proof:**
  - Let: $\boldsymbol{a} = |\boldsymbol{A}|, \boldsymbol{b} = |\boldsymbol{B}|$ and $\boldsymbol{e} =$ # edges from **A** to **B**
  - Enough to choose some $\boldsymbol{x_i}$ based on **A** and **B** such that:

$$\lambda_2 \leq \underbrace{\frac{\sum (x_i - x_j)^2}{\sum_i x_i^2}}_{\lambda_2 \text{ is only smaller}} \leq 2\alpha \qquad \text{(while also } \textstyle\sum_i x_i = 0\text{)}$$

Approx. Guarantee of Spectral

Details!

- **Proof (continued):**
  - **1) Let's set:** $\boldsymbol{x_i} = \begin{cases} -\frac{\mathbf{1}}{\boldsymbol{a}} & \boldsymbol{if\ i \in A} \\ +\frac{\mathbf{1}}{\boldsymbol{b}} & \boldsymbol{if\ i \in B} \end{cases}$

    Note: |A|<|B|

    - Let's quickly verify that $\sum_i x_i = 0$: $a\left(-\frac{1}{a}\right) + b\left(\frac{1}{b}\right) = \mathbf{0}$
  - **2) Then:** $\frac{\sum(x_i - x_j)^2}{\sum_i x_i^2} = \frac{\sum_{i \in A, j \in B}\left(\frac{1}{b}+\frac{1}{a}\right)^2}{a\left(-\frac{1}{a}\right)^2 + b\left(\frac{1}{b}\right)^2} = \frac{e \cdot \left(\frac{1}{a}+\frac{1}{b}\right)^2}{\frac{1}{a}+\frac{1}{b}} =$

$$e\left(\frac{1}{a}+\frac{1}{b}\right) \le e\left(\frac{1}{a}+\frac{1}{a}\right) = \boldsymbol{e}\frac{\mathbf{2}}{\boldsymbol{a}} \le \mathbf{2}\boldsymbol{\alpha}$$

e … number of edges between A and B

Which proves that the cost achieved by spectral is better than twice the OPT cost

Approx. Guarantee of Spectral

Details!

- **Putting it all together: The Cheeger inequality**

$$\frac{\alpha^2}{2k_{max}} \leq \lambda_2 \leq 2\alpha$$

  - where k_{max} is the maximum node degree in the graph
    - Note we only provide the 1st part: $\lambda_2 \leq 2\alpha$
    - We did not prove $\frac{\alpha^2}{2k_{max}} \leq \lambda_2$
  - Overall this always certifies that λ_2 always gives a useful bound

So far…

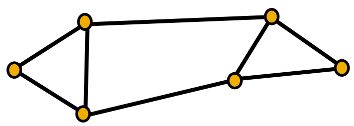
- **How to define a "good" partition of a graph?**
  - Minimize a given graph cut criterion
- **How to efficiently identify such a partition?**
  - Approximate using information provided by the eigenvalues and eigenvectors of a graph
- **Spectral Clustering**

Spectral Clustering Algorithm

- **Three basic stages:**
  - **1) Pre-processing**
    - Construct a matrix representation of the graph
  - **2) Decomposition**
    - Compute eigenvalues and eigenvectors of the matrix
    - Map each point to a lower-dimensional representation based on one or more eigenvectors
  - **3) Grouping**
    - Assign points to two or more clusters, based on the new representation

Spectral Partitioning Algorithm

- **1) Pre-processing:**
  - Build Laplacian matrix L of the graph



	1	2	3	4	5	6
1	3	-1	-1	0	-1	0
2	-1	2	-1	0	0	0
3	-1	-1	3	-1	0	0
4	0	0	-1	3	-1	-1
5	-1	0	0	-1	3	-1
6	0	0	0	-1	-1	2

- **2) Decomposition:**
  - Find eigenvalues λ and eigenvectors x of the matrix L
  - Map vertices to corresponding components of x_2

λ=

0.0
1.0
3.0
3.0
4.0
5.0

X =

0.4	0.3	-0.5	-0.2	-0.4	-0.5
0.4	0.6	0.4	-0.4	0.4	0.0
0.4	0.3	0.1	0.6	-0.4	0.5
0.4	-0.3	0.1	0.6	0.4	-0.5
0.4	-0.3	-0.5	-0.2	0.4	0.5
0.4	-0.6	0.4	-0.4	-0.4	0.0

1	0.3
2	0.6
3	0.3
4	-0.3
5	-0.3
6	-0.6

How do we now find the clusters?

Spectral Partitioning

- 3) **Grouping:**
  - Sort components of reduced 1-dimensional vector
  - Identify clusters by splitting the sorted vector in two
- **How to choose a splitting point?**
  - Naïve approaches:
    - Split at **0** or median value
  - More expensive approaches:
    - Attempt to minimize normalized cut in 1-dimension (sweep over ordering of nodes induced by the eigenvector)

1	0.3
2	0.6
3	0.3
4	-0.3
5	-0.3
6	-0.6

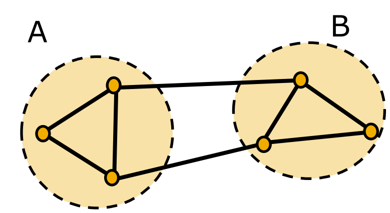
Split at 0:

Cluster A: Positive points

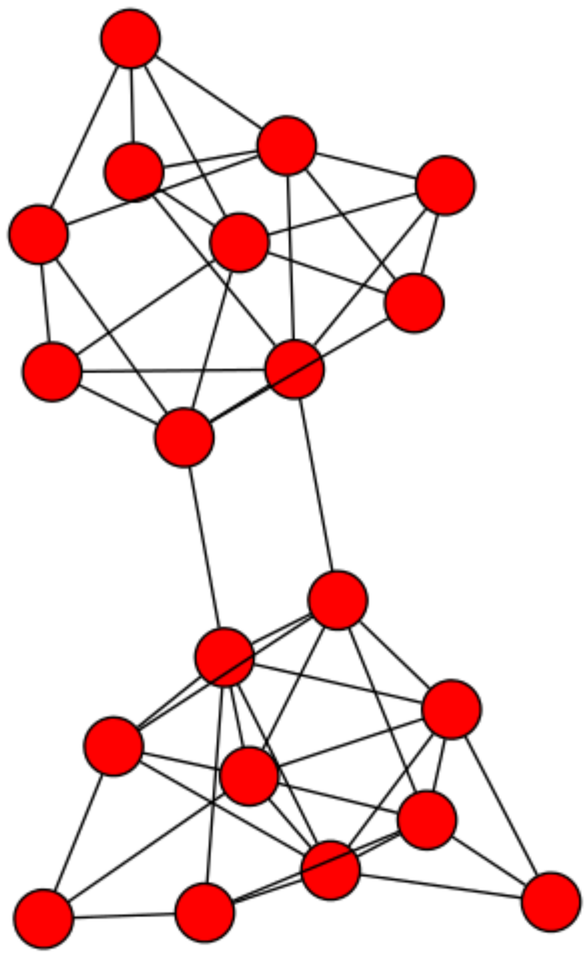
Cluster B: Negative points

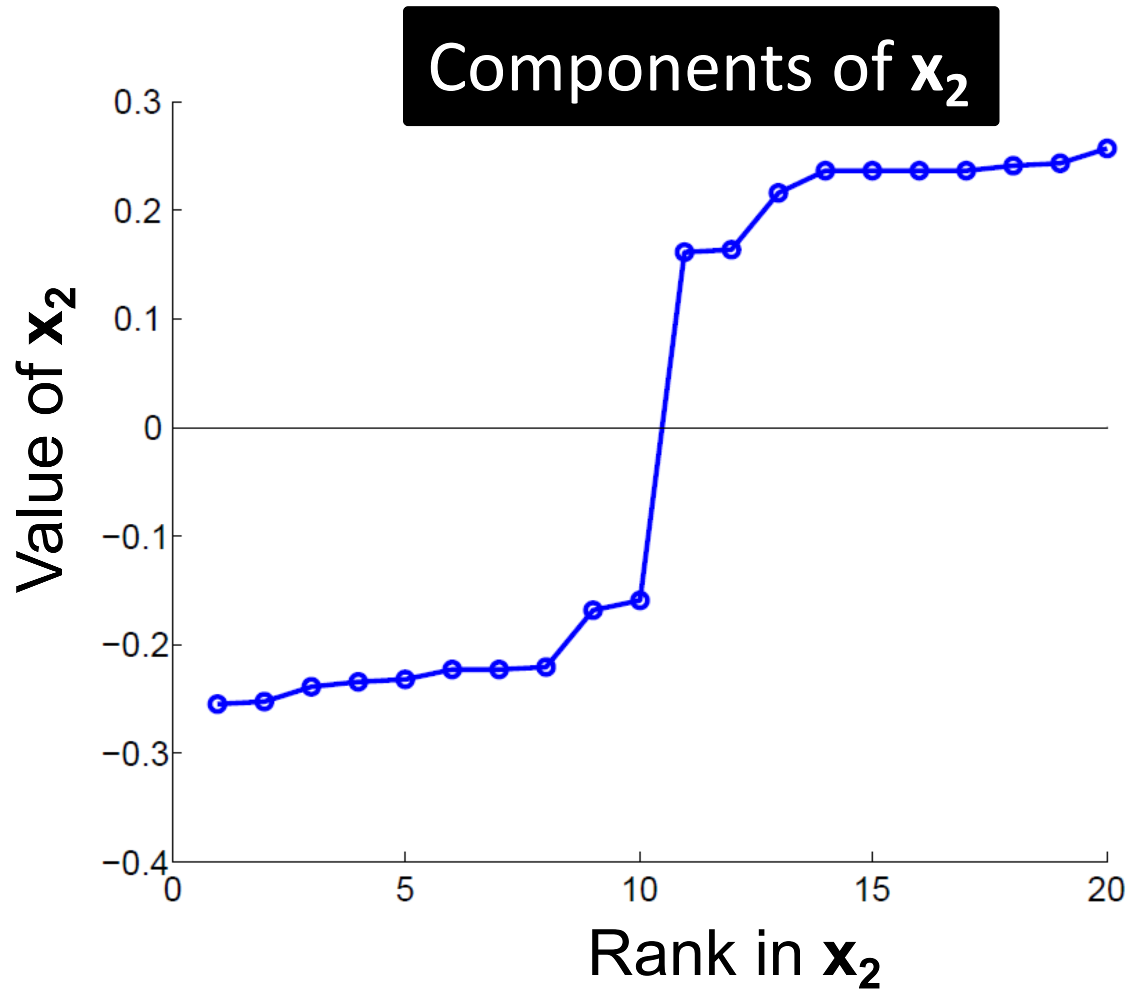
1	0.3
2	0.6
3	0.3

4	-0.3
5	-0.3
6	-0.6

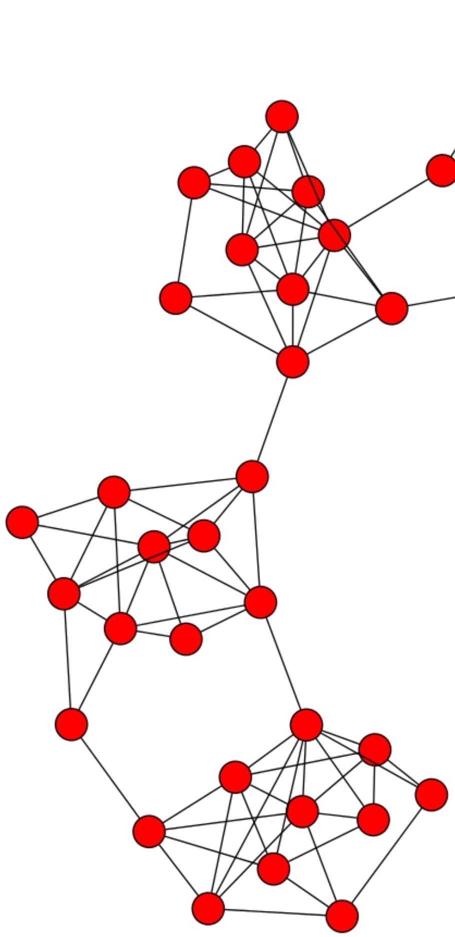


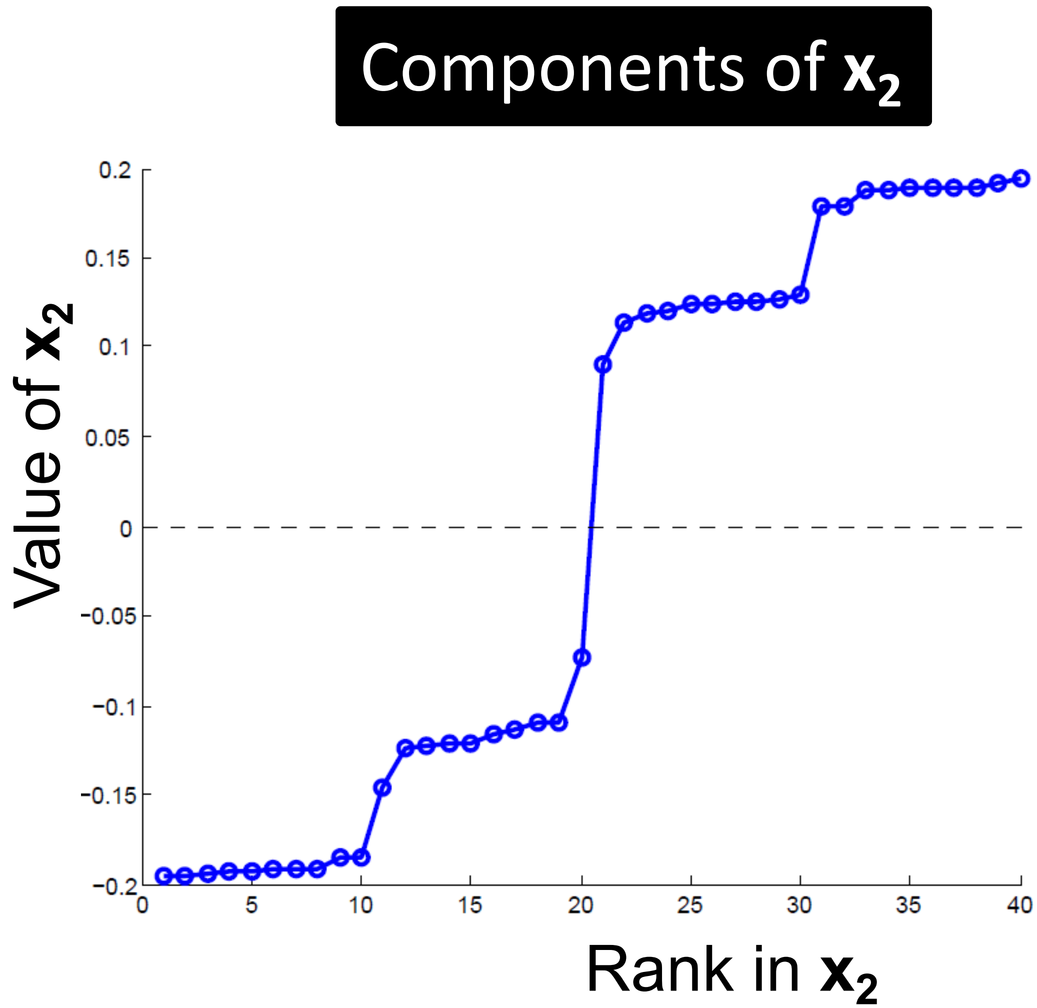
Example: Spectral Partitioning



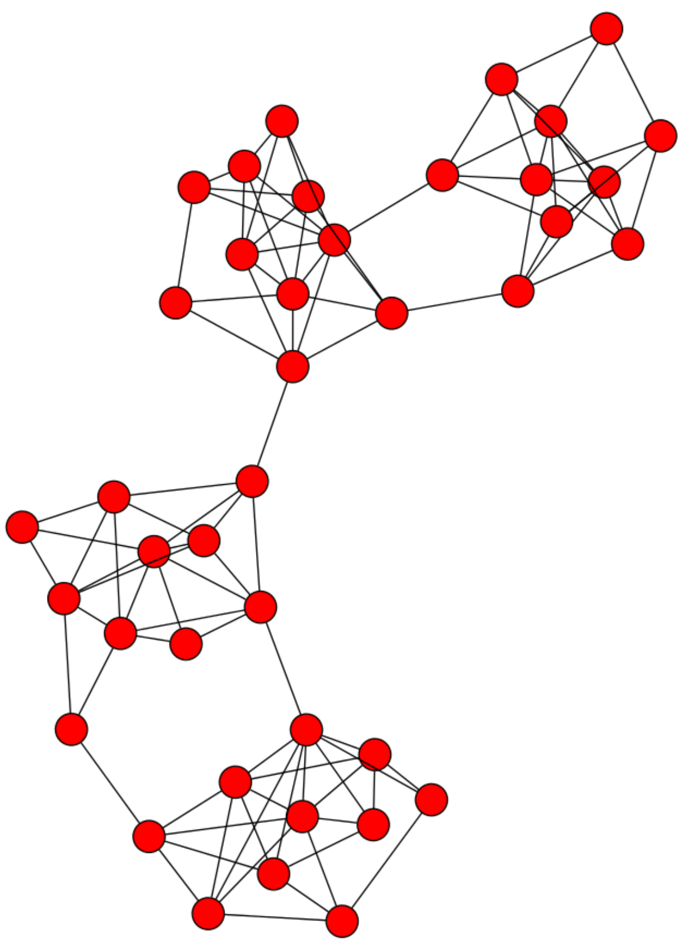


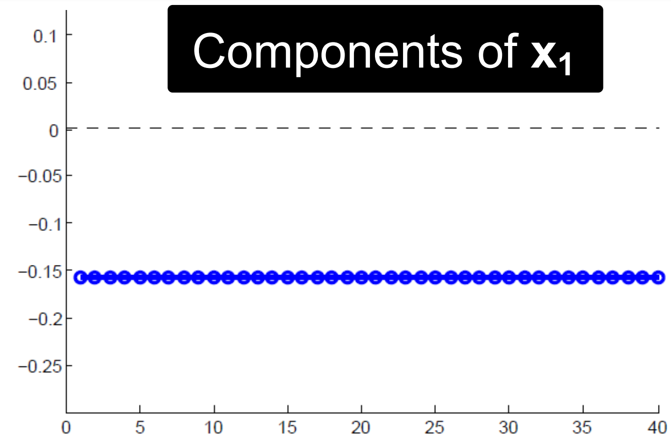
Example: Spectral Partitioning

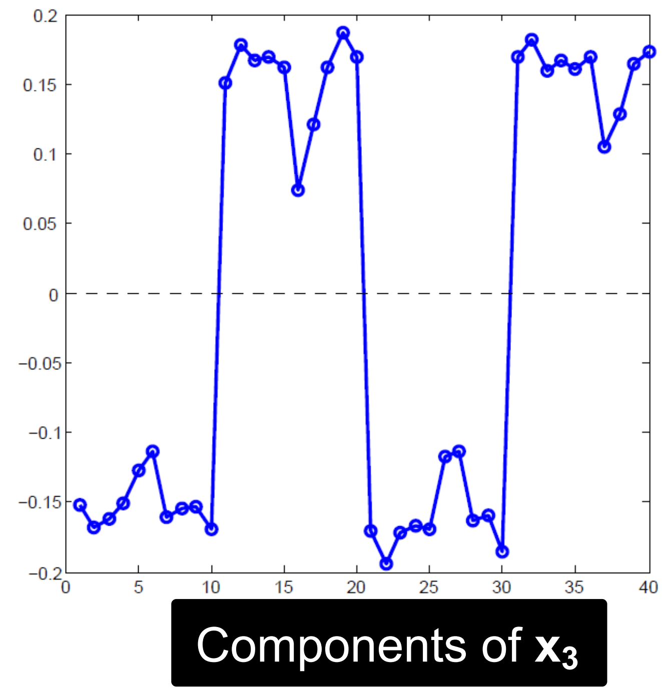




Example: Spectral partitioning







k-Way Spectral Clustering

- **How do we partition a graph into k clusters?**
- **Two basic approaches:**
  - **Recursive bi-partitioning** [Hagen et al., '92]
    - Recursively apply bi-partitioning algorithm in a hierarchical divisive manner
    - Disadvantages: Inefficient, unstable
  - **Cluster multiple eigenvectors** [Shi-Malik, '00]
    - Build a reduced space from multiple eigenvectors
      - Each node is now represented by $\boldsymbol{k}$ numbers
      - We then cluster (apply k-means) the nodes based on their $\boldsymbol{k}$-dim representation
    - Commonly used in recent papers
    - A preferable approach…

Why use multiple eigenvectors?

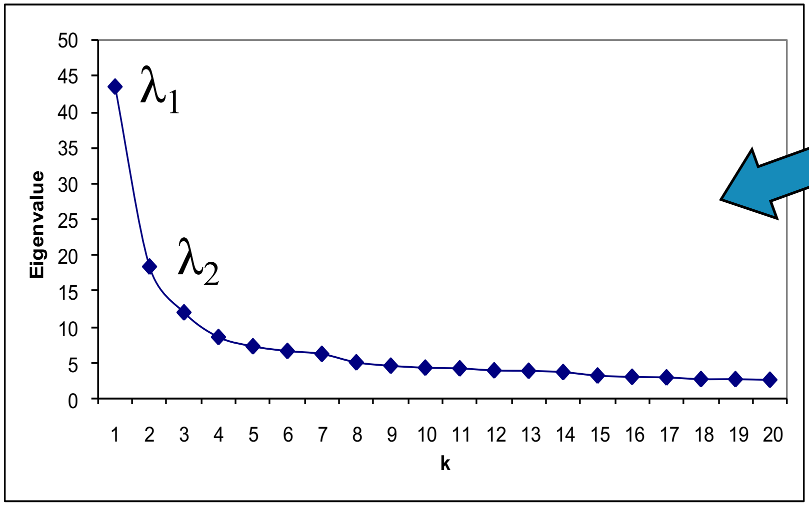
- **Approximates the optimal cut** [Shi-Malik, '00]
  - Can be used to approximate optimal k-way normalized cut
- **Emphasizes cohesive clusters**
  - Increases the unevenness in the distribution of the data
  - Associations between similar points are amplified, associations between dissimilar points are attenuated
  - The data begins to "approximate a clustering"
- **Well-separated space**
  - Transforms data to a new "embedded space", consisting of $\boldsymbol{k}$ orthogonal basis vectors
- Multiple eigenvectors prevent instability due to information loss

How to select k?

- **Eigengap:**
  - The difference between two consecutive eigenvalues
- **Most stable clustering is generally given by the value k that maximizes eigengap Δ_k:**

$$\Delta_k = |\lambda_k - \lambda_{k-1}|$$

- **Example:**



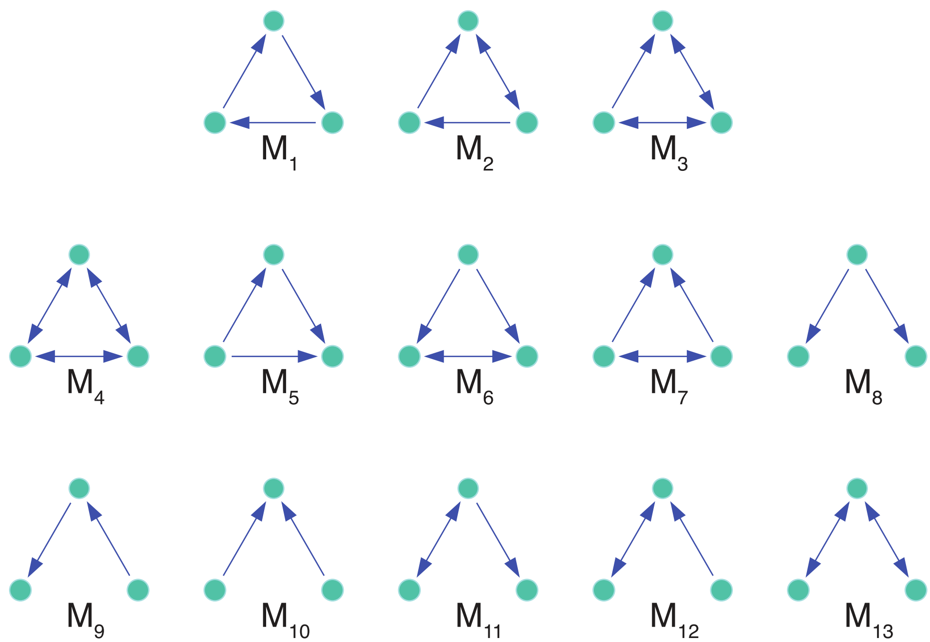
$$\max \Delta_k = |\lambda_2 - \lambda_1|$$

$\Rightarrow$ **Choose $k = 2$**

Motif-Based Spectral Clustering

Motif-based spectral clustering

- **What if we want our clustering based on other patterns (not edges)?**

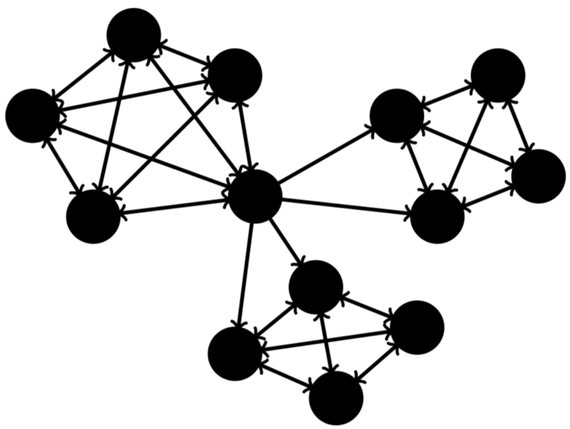


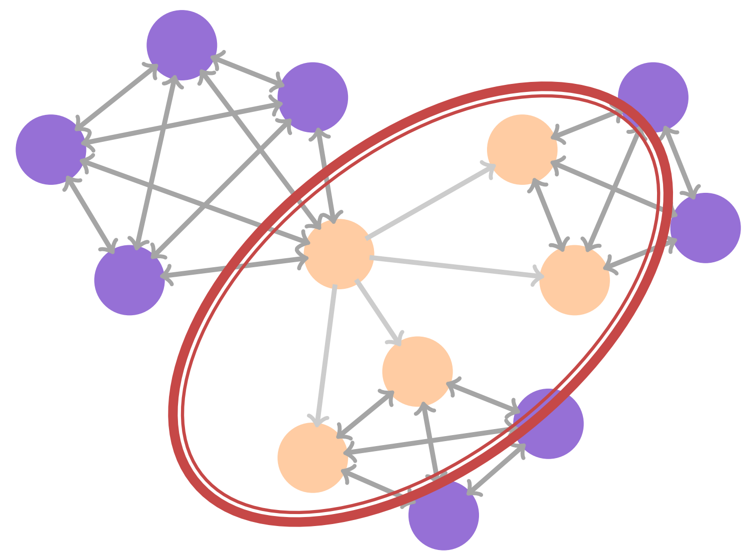
Small subgraphs (motifs, graphlets) are building blocks of networks [Milo et al., '02]

Topic 1: Modules of Motifs

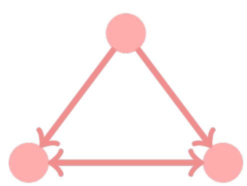
Find modules based on motifs!

Network:

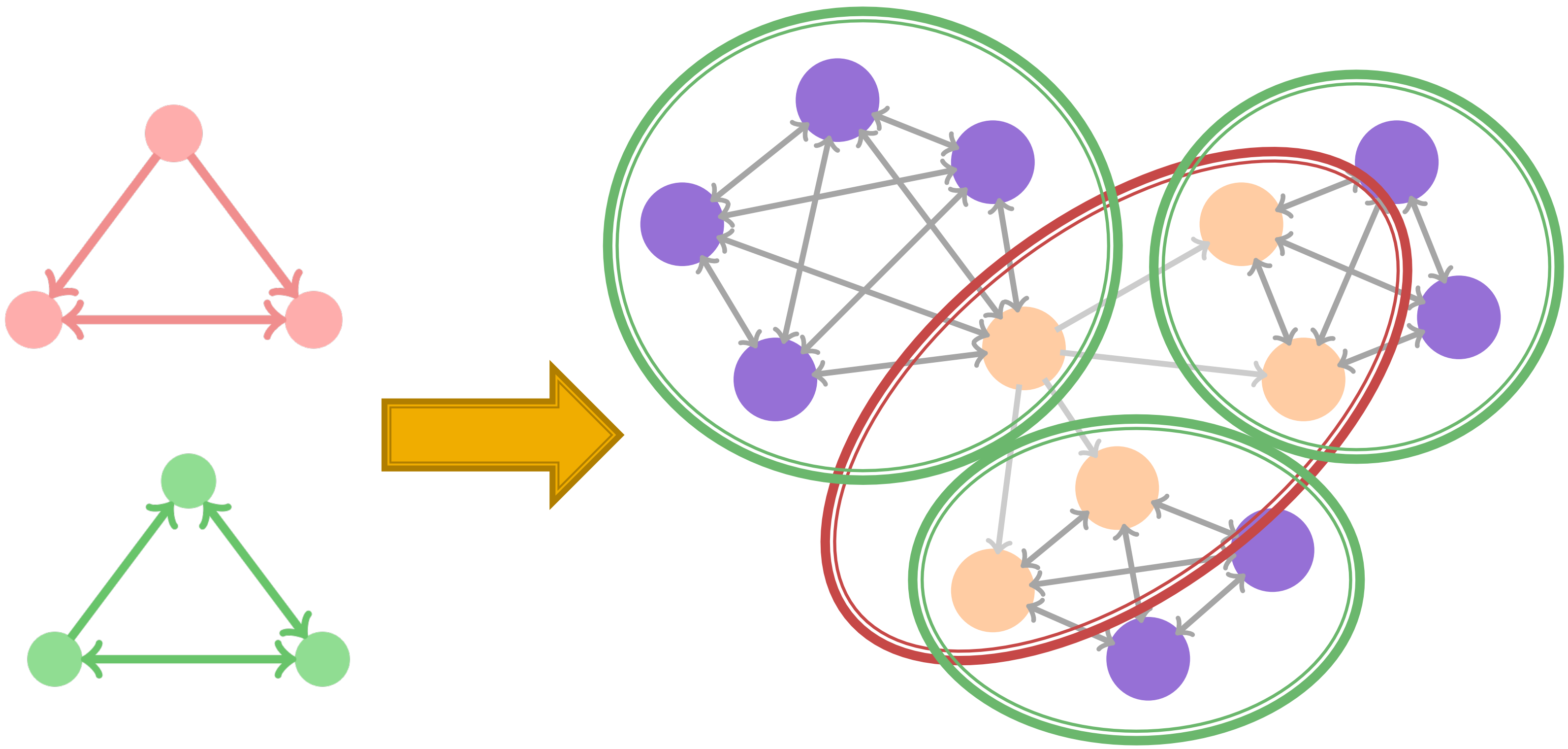




Motif:



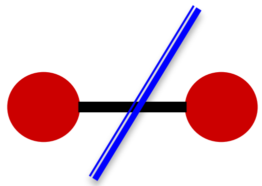
Modules of Motifs

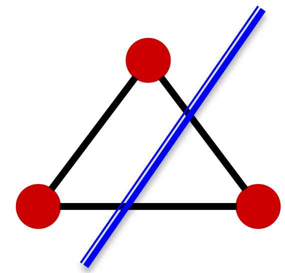


Different motifs reveal different modular structures!

Defining Motif Conductance

Generalize Cut and Volume to motifs:

$edges\ cut$ 

$motifs\ cut$ 

$vol(S) = $ #(edge end-points in S)

$vol_M(S) = $ #(motif end-points in S)

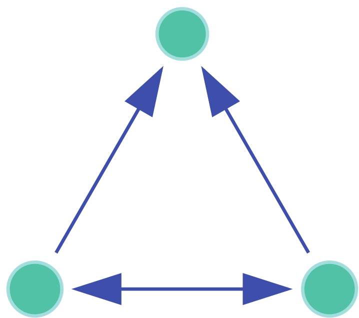
$$\phi(S) = \frac{\#(edges\ cut)}{vol(S)}$$

$$\boxed{\phi(S) = \frac{\#(motifs\ cut)}{vol_M(S)}}$$

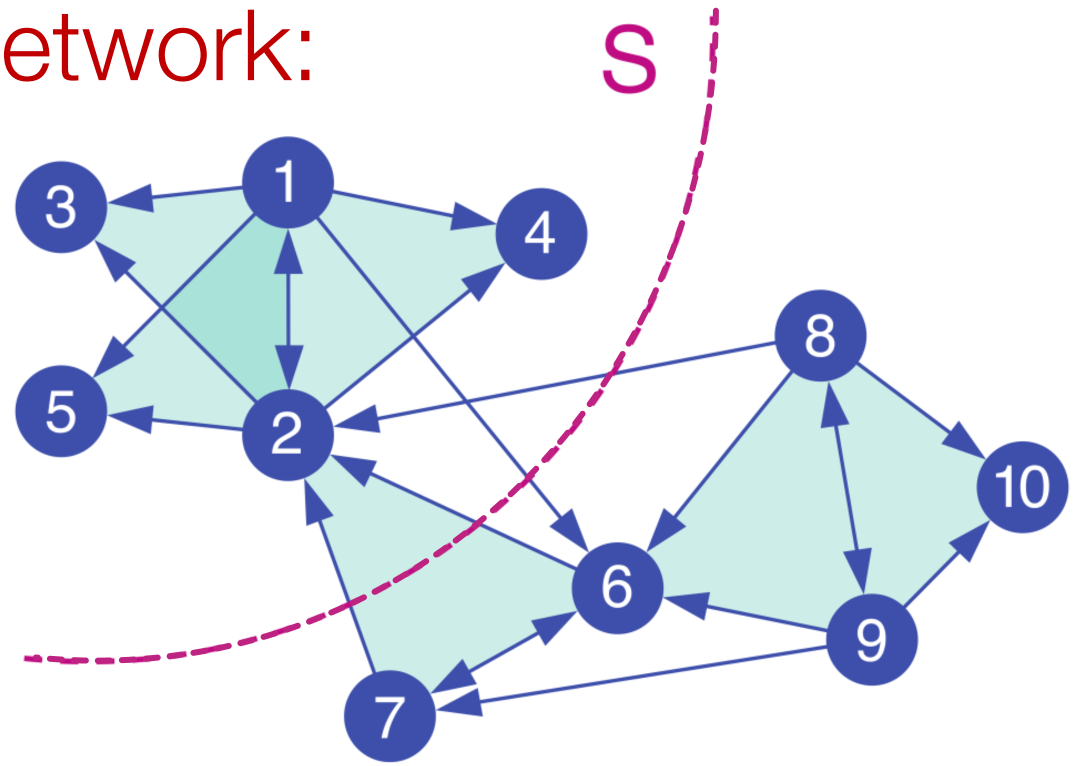
[Benson, Gleich, Leskovec, Science, 2016]

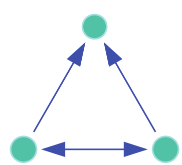
Motif Conductance: Example

Motif:



Network:



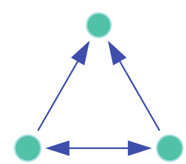


$$\phi_M(S) = \frac{\text{motifs cut}}{\text{motif volume}}$$

Higher-order Partitioning

How do we find clusters of motifs?

- Given a motif M and a graph G
- Find a set of nodes S that minimizes motif conductance



$$\phi_M(S) = \frac{\text{motifs cut}}{\text{motif volume}}$$

Bad news: Finding set S with the minimal motif conductance is NP-hard!

Motif Spectral Clustering

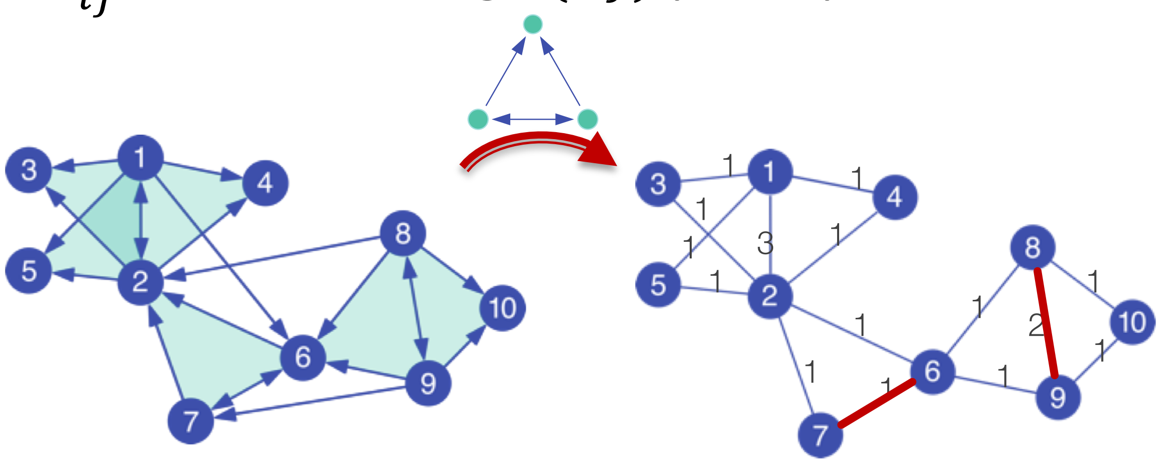
Solution: Motif Spectral Clustering

- Input: Graph $\boldsymbol{G}$ and motif $\boldsymbol{M}$
- Using $\boldsymbol{G}$ form a new weighted graph $\boldsymbol{W}^{(\boldsymbol{M})}$
- Apply spectral clustering on $\boldsymbol{W}^{(\boldsymbol{M})}$
- Output the clusters

Theorem: Resulting clusters will obtain near optimal motif conductance

Optimizing Motif Conductance

- **Three steps:**
  - **1) Pre-processing**
    - $W_{ij}^{(M)}$ = # times edge (i, j) participates in the motif M



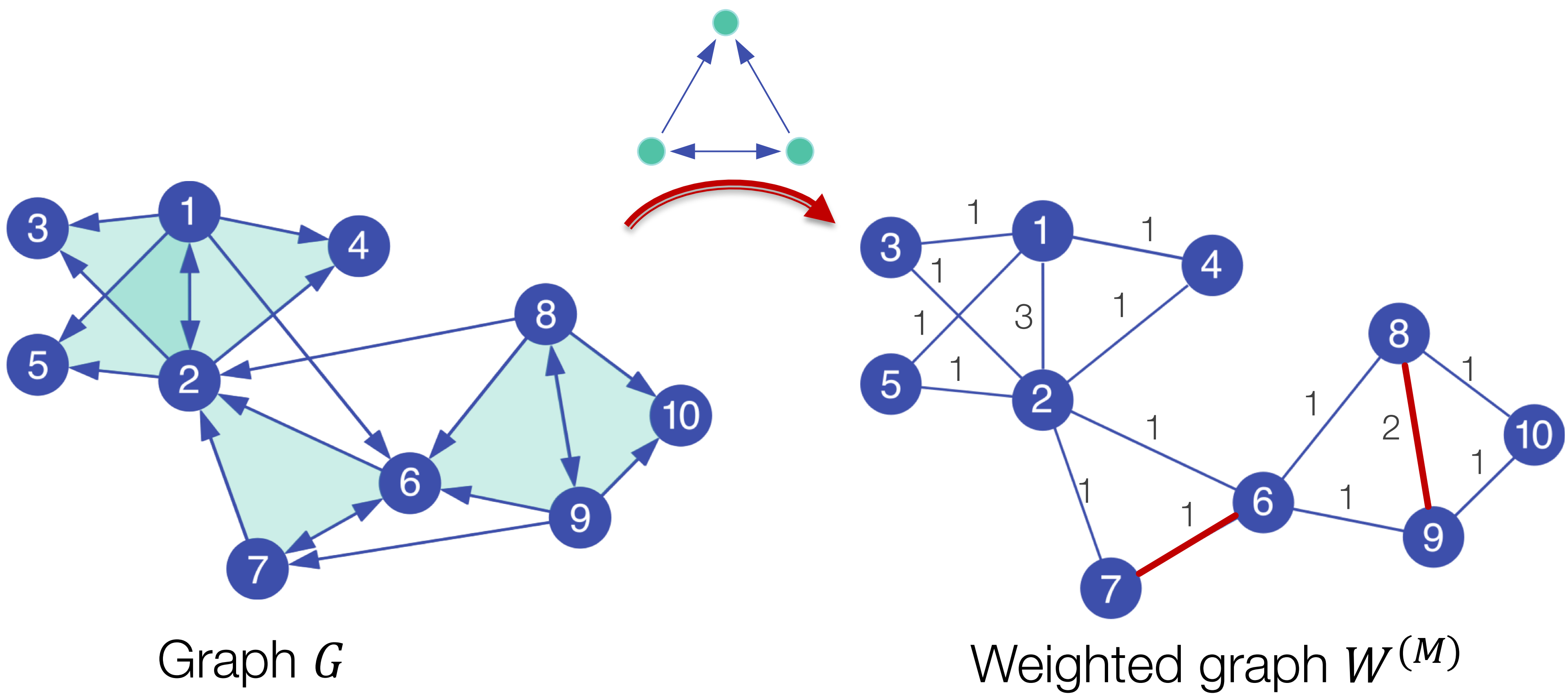
Graph G

Weighted graph W^(M)

See lecture 5 on motifs and the ESU algorithm for enumerating them

  - **2) Decomposition**
    - Use standard spectral clustering (but on $W^{(M)}$)
  - **3) Grouping**
    - Same as standard spectral clustering

Motif Spectral Clustering

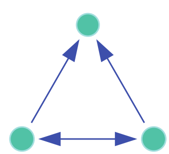


$W_{ij}^{(M)}$ = # of times edge (i,j) participates in motif M

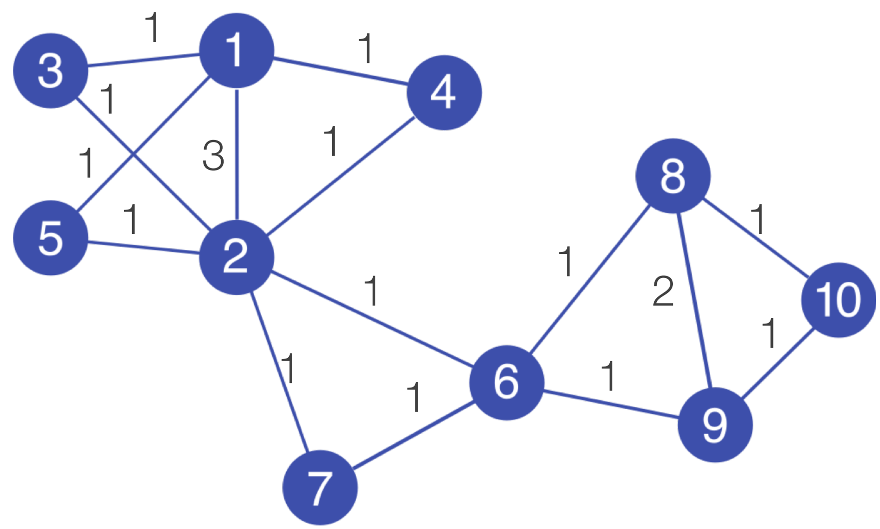
Motif Spectral Clustering

Insight:

Spectral clustering on weighted graph $W^{(M)}$ finds clusters of low motif conductance:



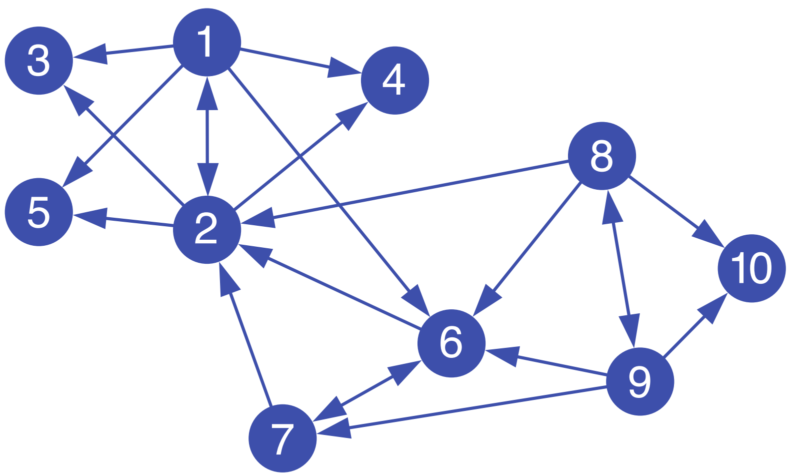
$$\phi_M(S) = \frac{\text{motifs cut}}{\text{motif volume}}$$



Weighted graph $W^{(M)}$

$W_{ij}^{(M)}$ = # of times edge (i,j) participates in motif M

Step 1: Create W



$$
\text{Nodes}\quad
\begin{array}{c}
\text{Nodes} \\
\begin{array}{r c}
 & \begin{array}{cccccccccc} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{array} \\
\begin{array}{r} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{array} &
\begin{bmatrix}
0 & \mathbf{3} & 1 & 1 & 1 & 0 & 0 & 0 & 0 & 0 \\
\mathbf{3} & 0 & 1 & 1 & 1 & 1 & 1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 & 0 & 0 & 1 & 1 & 1 & 0 \\
0 & 1 & 0 & 0 & 0 & 1 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & 0 & \mathbf{2} & 1 \\
0 & 0 & 0 & 0 & 0 & 1 & 0 & \mathbf{2} & 0 & 1 \\
0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 & 1 & 0
\end{bmatrix}
\end{array}
\end{array}
$$

Step 1: Given motif M. Form weighted graph $W^{(M)}$

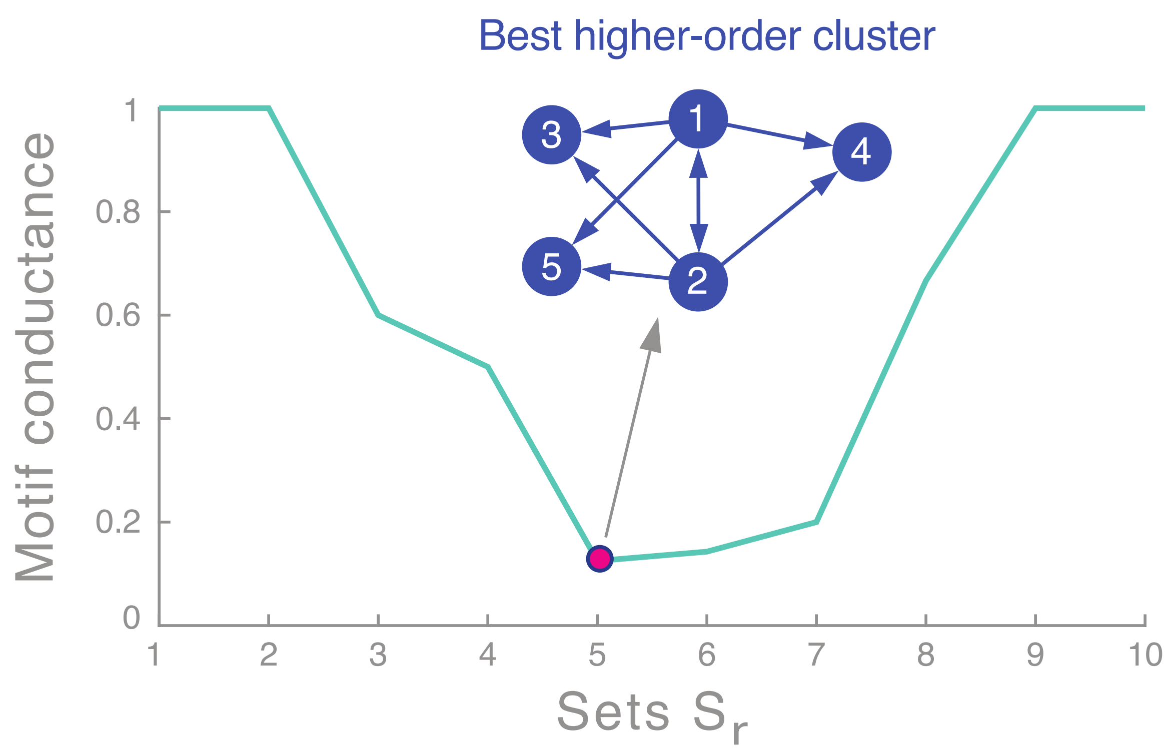
Step 2: Apply Spectral Clust to $W^{(M)}$

Step 2: Apply spectral clustering:
Compute Fiedler vector $f^{(M)}$
associated with λ_2 of the Laplacian of $L^{(M)}$

Set: $L^{(M)} = D - W^{(M)}$
Compute: $L^{(M)} f^{(M)} = \lambda_2 f^{(M)}$
Use $f^{(M)}$ to identify communities

Degree matrix
$$D_{ii} = \sum_j W_{ij}^{(M)}$$

Step 3: Grouping (Sweep Procedure)



Step 3: Sort nodes by values in $f^{(M)}$: $f_1, f_2, \ldots f_n$

Let $S_r = \{f_1, \ldots, f_r\}$ and compute the motif conductance of each S_r

Motif Cheeger Inequality

Theorem: The algorithm finds a set of nodes S for which

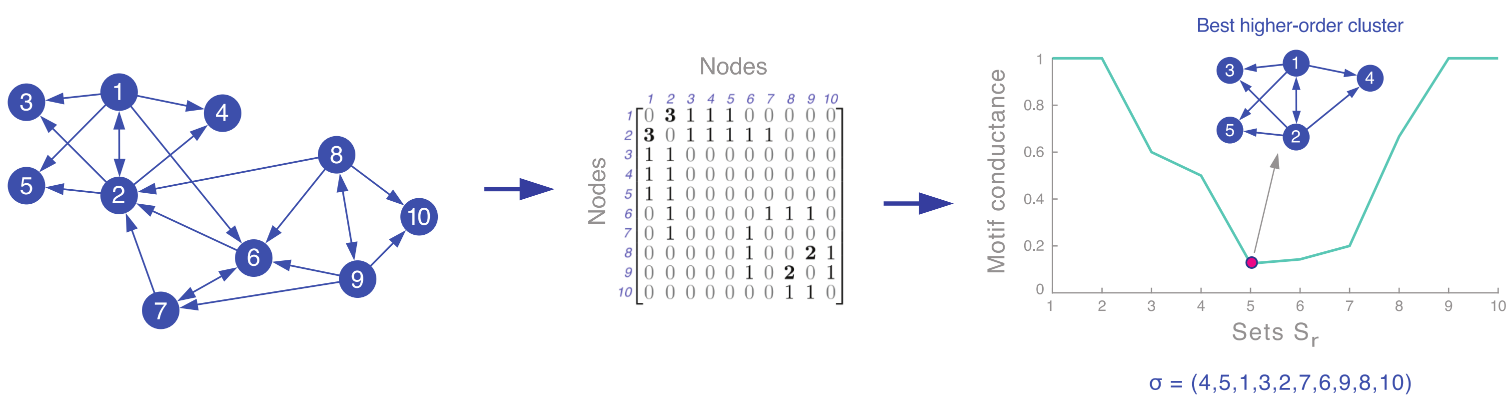
$$\phi_M(S) \leq 4\sqrt{\phi_M^*}$$

$\phi_M(S)$… motif conductance of S found by our algorithm
ϕ_M^* … motif conductance of optimal set S*

In other words: Clusters S found by the method are provably near optimal

Summary

- Generalization of community detection to higher-order structures
- Motif-conductance objective admits a motif Cheeger inequality
- Simple, fast, and scalable:



Two Examples

1) We don’t know a motif of interest

- Food webs and new applications

2) We know the motif of interest

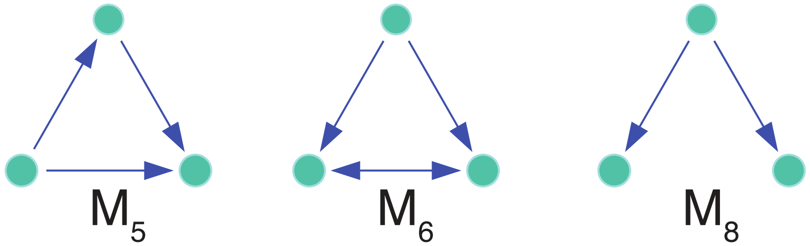
- Regulatory transcription networks, connectome, social networks

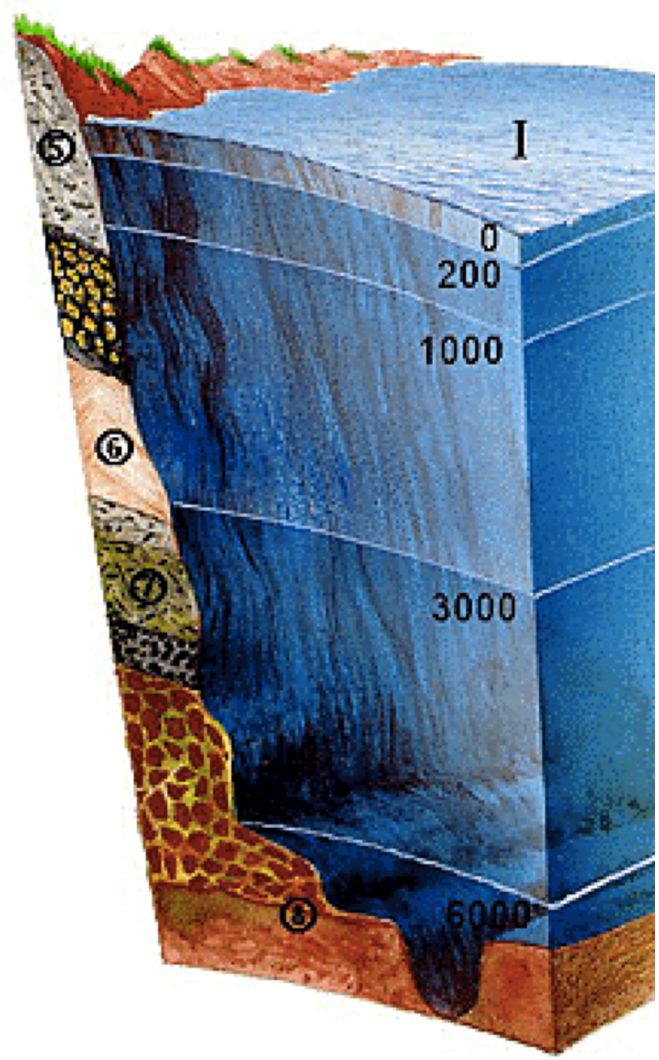
Application 1: Food webs

Florida Bay food web:

- **Nodes:** species in the ecosystem
- **Edges:** carbon exchange (who eats whom)

Different motifs capture different energy flow patterns:





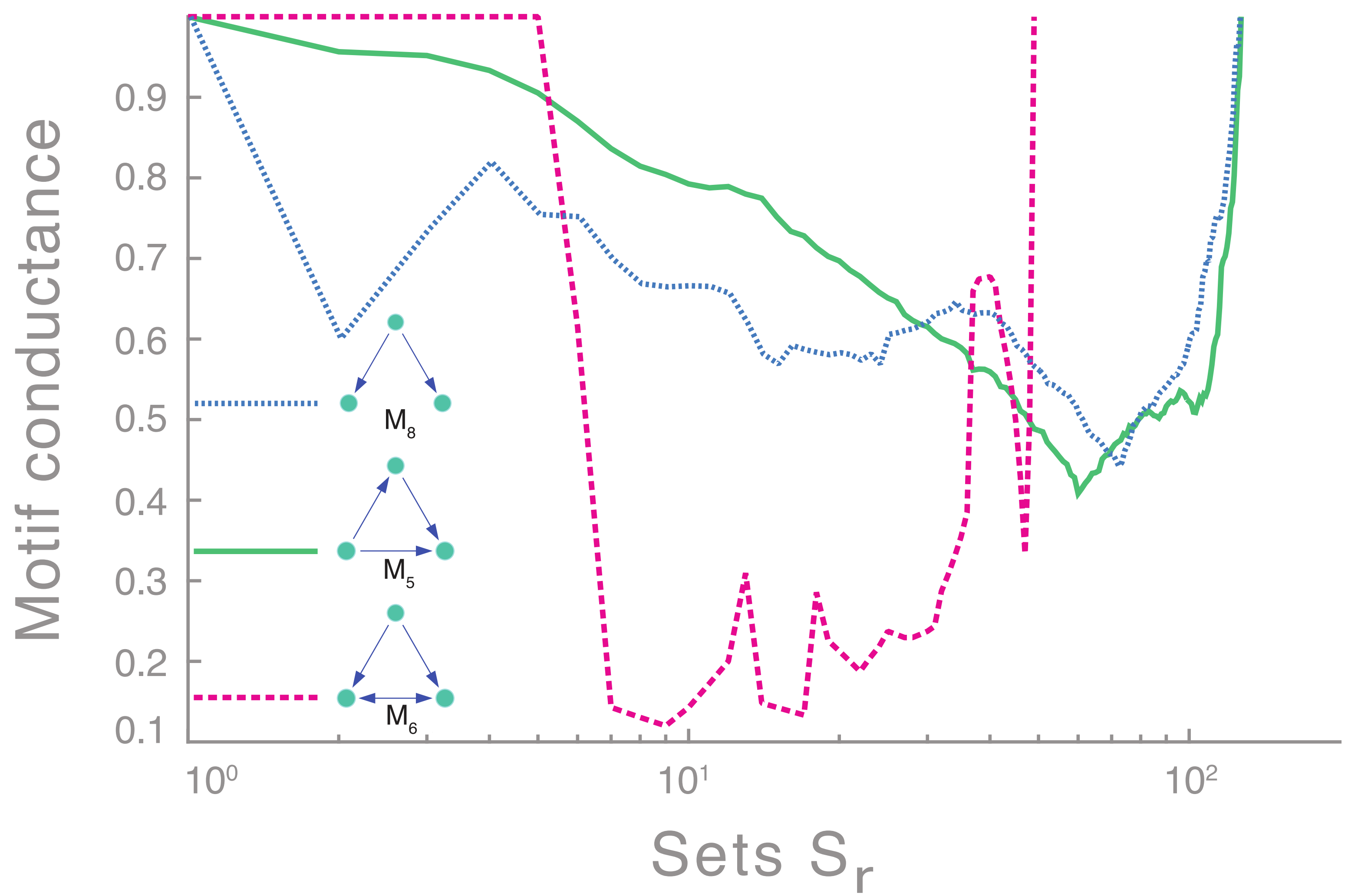
Florida Bay Food Web

Which motif organizes the food web?

Approach:

- Run motif spectral clustering separately for each of the 13 motifs
- Examine the **Sweep profile (next slide)** to see which motif gives best clusters

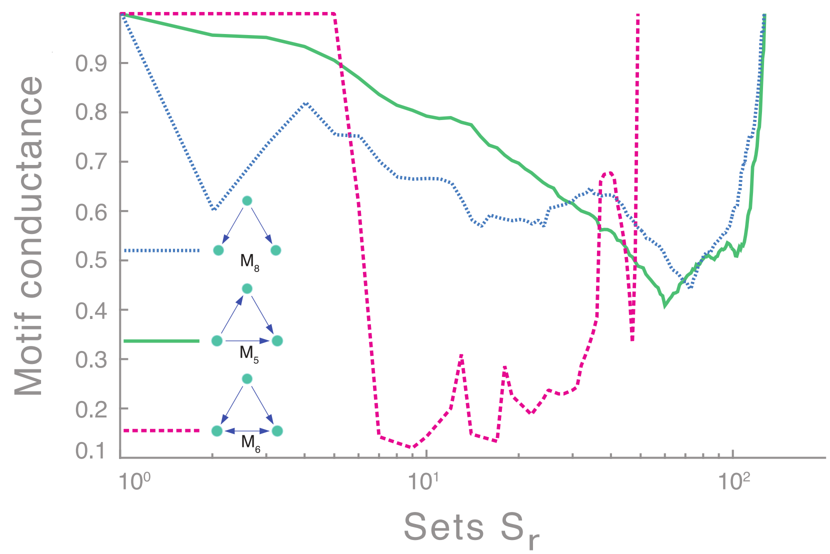
Florida Bay Food Web

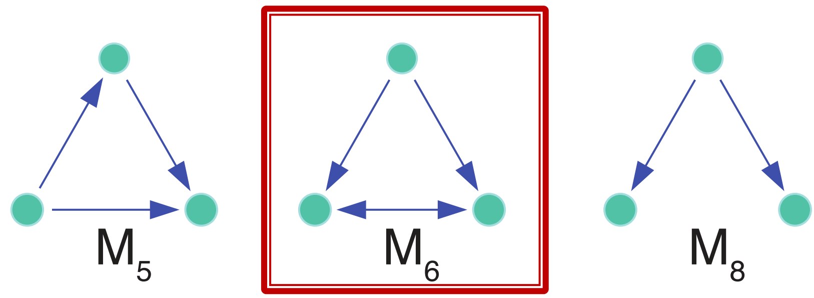


Food Web: Observations

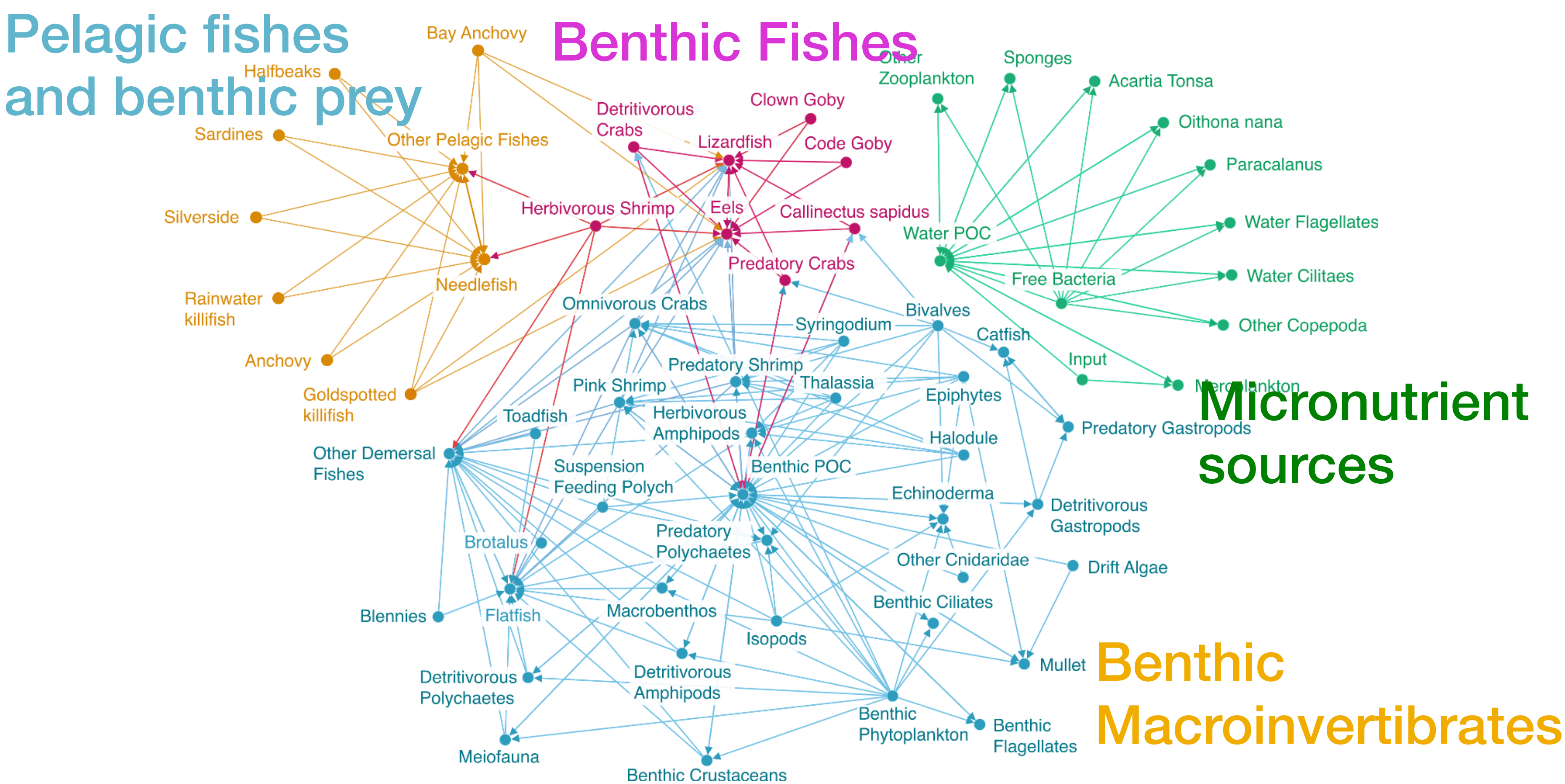
Observation:
Network organizes based on motif M_6 (but not M_5 or M_8)

- There exist good cuts for M_6 but not for M_5 or M_8



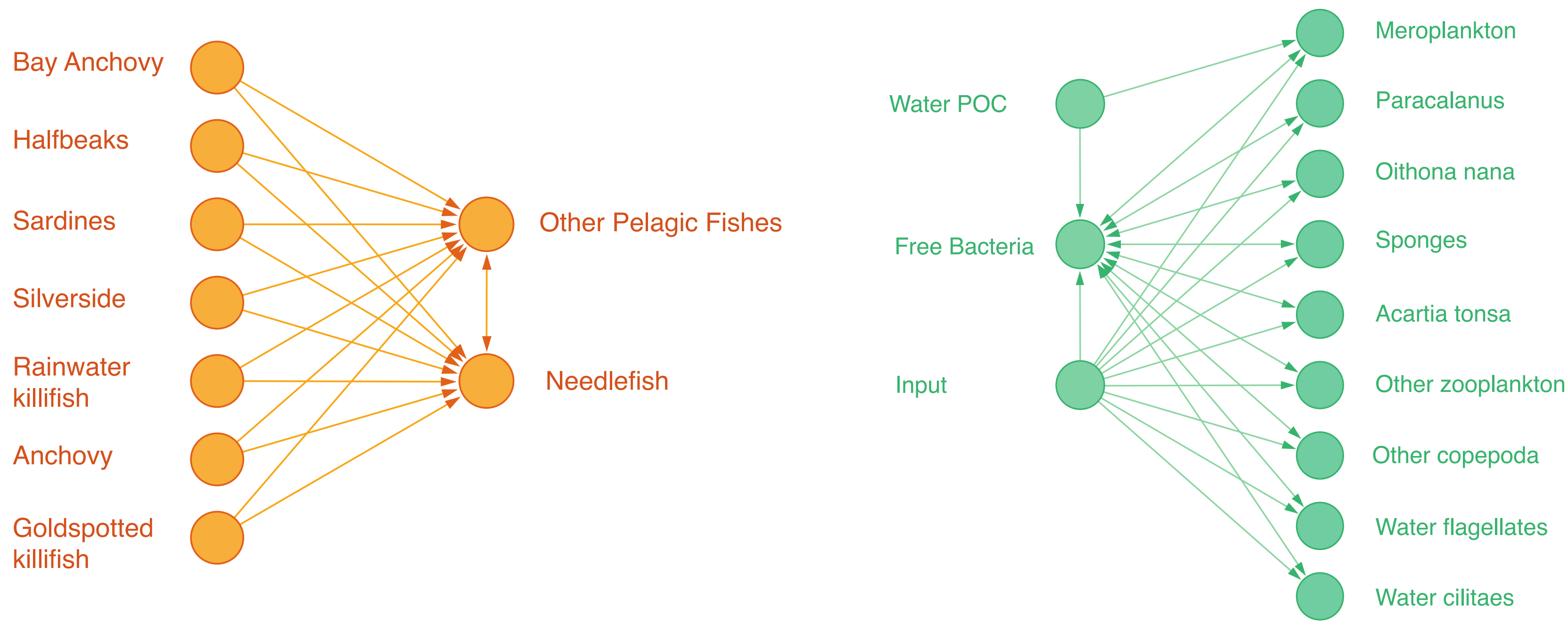


Food Web: Clusters



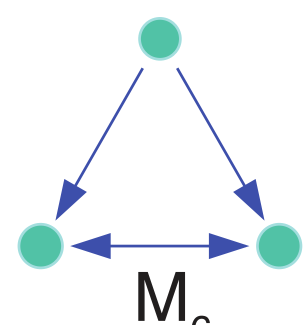
M_6 reveals known aquatic layers with higher accuracy (84% vs. 65%)

Structure of Aquatic Layers



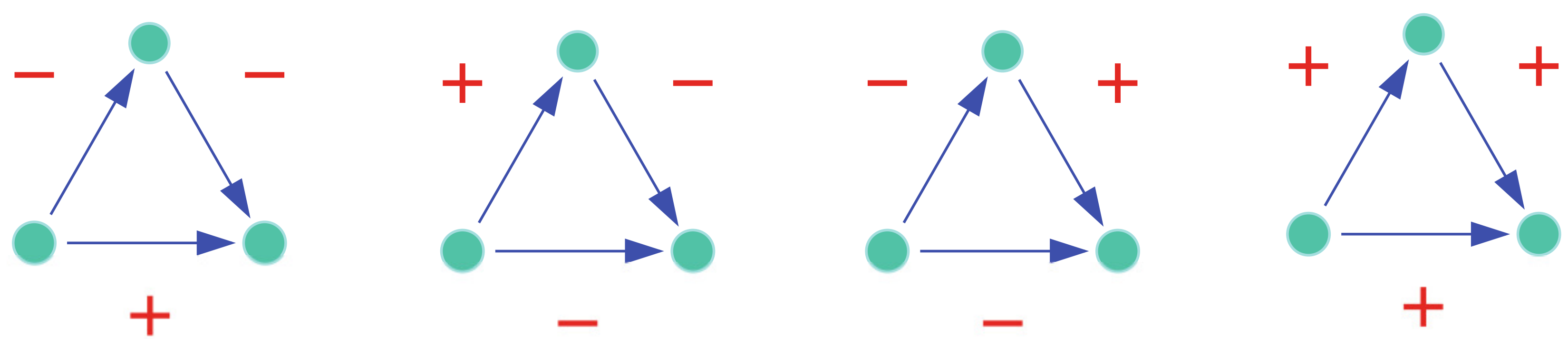
Aquatic layers organize based on M_6

- Many instances of M_6 inside
- Few instances of M_6 cross



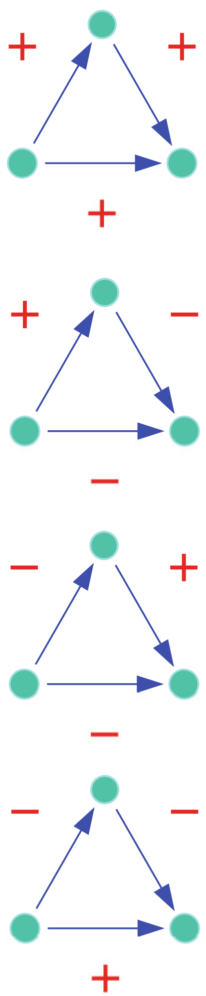
(2) Gene Regulatory Networks

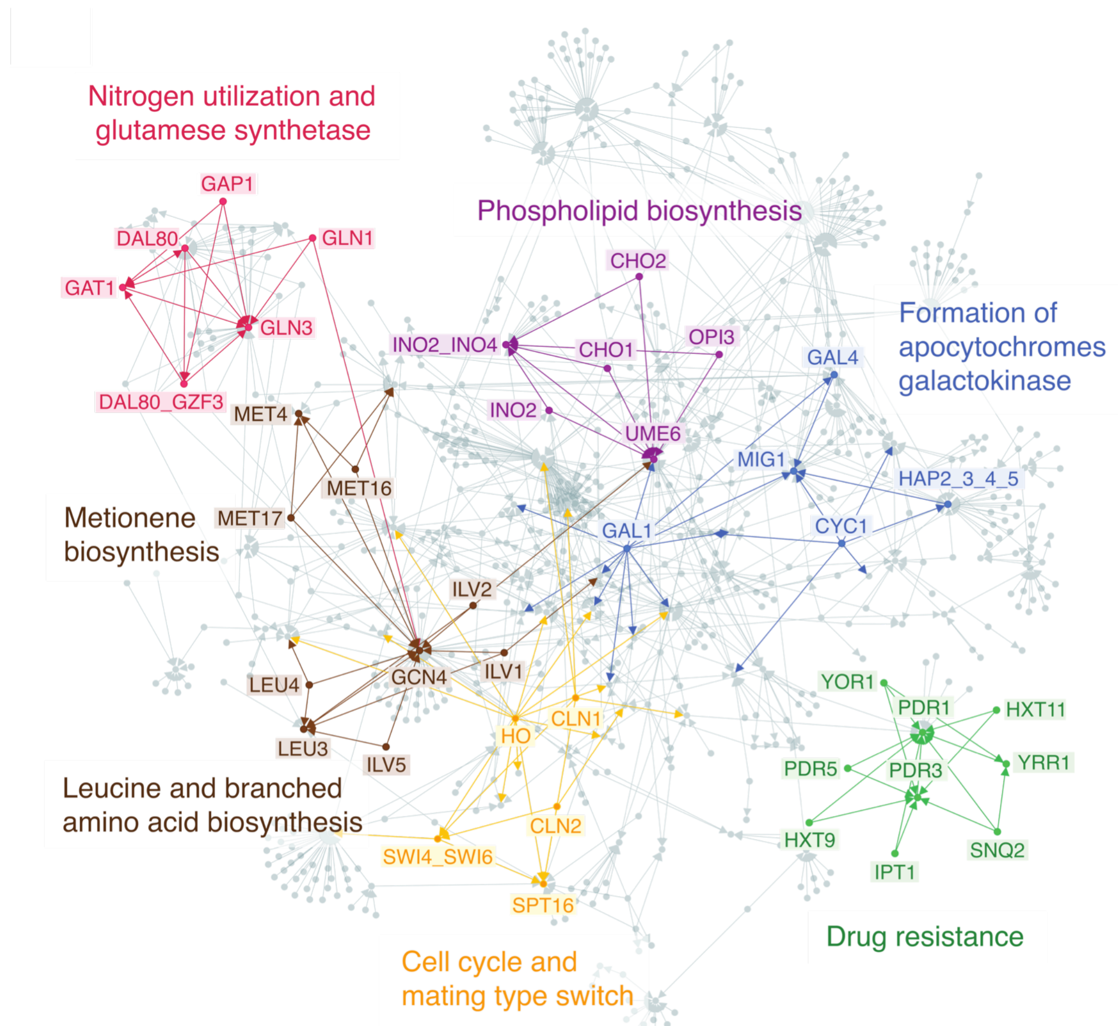
- Nodes are groups of genes in mRNA
- Edges are directed transcriptional regulation relationships



- The "feedforward loop" motif represents biological function [Alon '07]

Yeast Regulatory Network

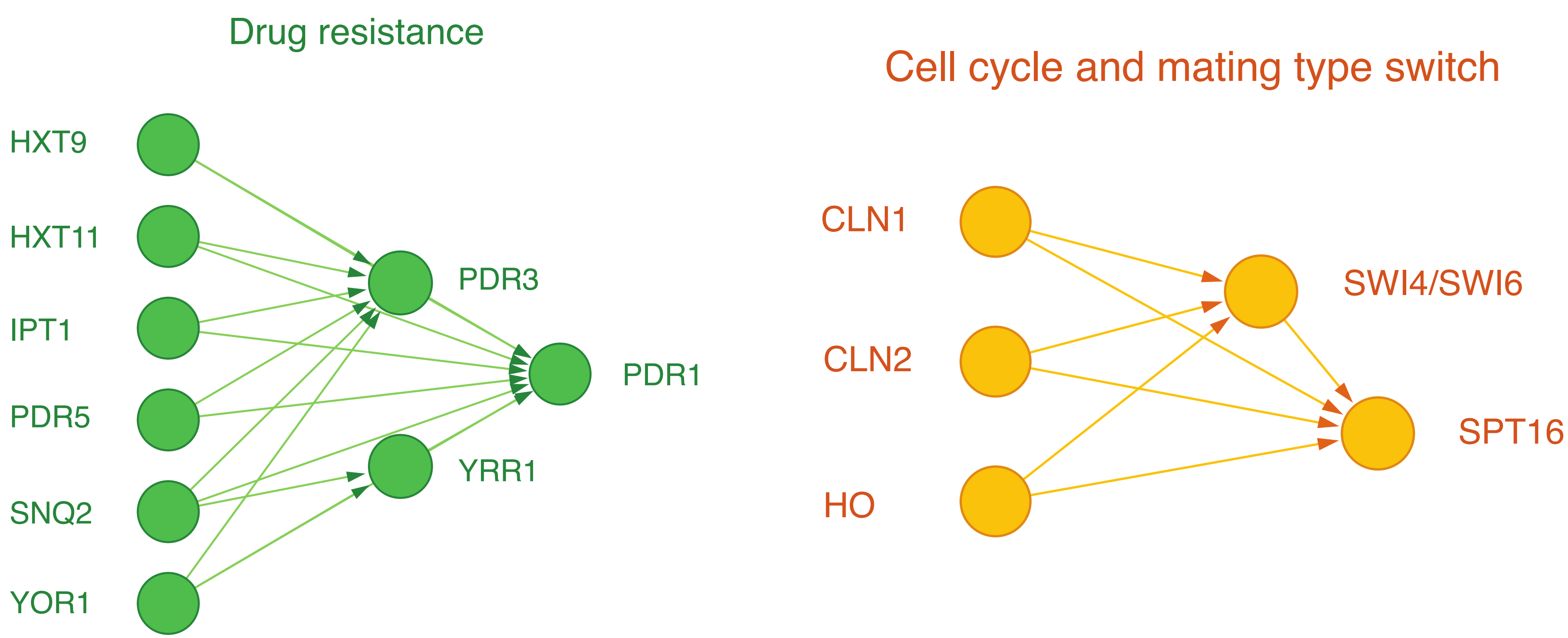




97% detection accuracy (vs. 68-82%)

Structure of Modules

- Feed forward loops:



Many other partitioning methods

- **METIS:**
  - Heuristic but works really well in practice
  - http://glaros.dtc.umn.edu/gkhome/views/metis
- **Graclus:**
  - Based on kernel k-means
  - http://www.cs.utexas.edu/users/dml/Software/graclus.html
- **Louvain:**
  - Based on Modularity optimization
  - http://perso.uclouvain.be/vincent.blondel/research/louvain.html
- **Clique percorlation method:**
  - For finding overlapping clusters
  - http://angel.elte.hu/cfinder/