# Spectral Clustering

## Part 2: Weighted Graph Laplacians

Ng Yen Kaow

# Minimum Cut Problem

- The minimum cut of an undirected graph $G = (V, E)$ is a partition of $V$ into two groups $S$ and $\bar{S}$ so that the number of edges between $S$ and $\bar{S}$ is minimized
  - Karger's algorithm finds an optimal solution in $O(|V|^2|E|\log|V|)$ time with probability $1/\binom{|V|}{2}$
- Recall that for the unnormalized $L = D - W$, $x^{\mathrm{T}}Lx$ = 4 times the number of adjacent vertices of different values in $x$
  - We showed in Part 1 that an $x$ which minimizes $x^{\mathrm{T}}Lx$ can be approximated from eigendecomposition
  - In fact, it added an (ineffective) balance requirement

# Minimum Bisection Problem

- The minimum bisection of an undirected graph $G = (V, E)$ is a partition of $V$ into two groups $S$ and $\bar{S}$ so that the number of edges between $S$ and $\bar{S}$ is minimized, under the constraint that $|S| = |\bar{S}|$ (or $\big||S| - |\bar{S}|\big| = 1$ for odd $|V|$)
- As in minimum cut, let $x_i = \begin{cases} 1 & \text{if } v_i \in S \\ -1 & \text{if } v_i \in \bar{S} \end{cases}$
  - In which case, $|S| = |\bar{S}|$ implies $\sum_i x_i = 0$, which implies $x \perp \mathbf{1}$ (or $x \perp b\mathbf{1}$ for any constant value $b$)

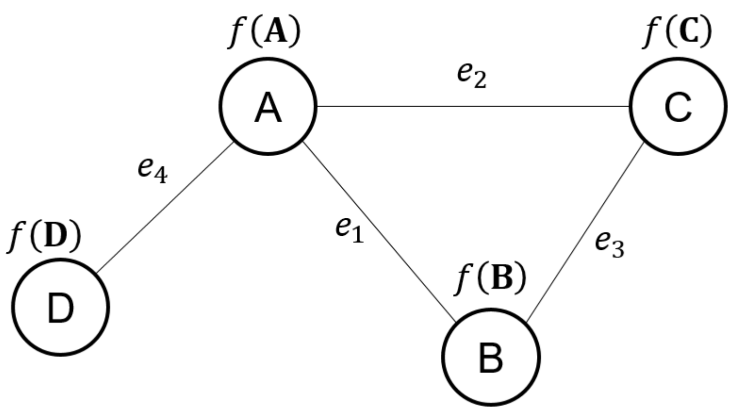
# Constrained optimization problem

- Minimize $x^{\mathrm{T}}Lx$ where $L = D - A$ subject to $x_i \in \{1, -1\}$ and $x^{\mathrm{T}}\mathbf{1} = 0$
  - $x_i \in \{1, -1\}$ and $x^{\mathrm{T}}\mathbf{1} = 0$ (that is, $x \perp \mathbf{1}$) together ensures balance in the partition
- Problem is NP-hard
- In contrast, eigendecomposition of an $|V| \times |V|$ matrix takes $O(|V|^3)$ time
  - Faster if only a few eigenpairs are needed, like in the case of spectral clustering

# Constrained optimization problem

- Minimize $x^{\mathrm{T}}Lx$ where $L = D - A$ subject to $x_i \in \{1, -1\}$ and $x^{\mathrm{T}}\mathbf{1} = 0$

- Example of cuts (shown with Rayleigh quotient for comparison later)




| Group 1 | Group 2 | $x^T Lx$ | $\frac{x^T Lx}{x^T x}$ |
|---|---|---|---|
| A | B C D | 12 | 3 |
| B | A C D | 8 | 2 |
| C | A B D | 8 | 2 |
| D | A B C | 4 | 1 |
| A B | C D | 12 | 3 |
| A C | B D | 12 | 3 |
| **A D** | **B C** | **8** | **2** |
| A B C D | ∅ | 0 | 0 |

# Relaxed Rayleigh quotient version

- Minimize $x^{\mathrm{T}}Lx$ where $L = D - A$ subject to $x^{\mathrm{T}}x = 1$ and $x^{\mathrm{T}}\mathbf{1} = 0$
  - $x^{\mathrm{T}}x = 1$ (or any constant)
    - Allows problem to be solved as minimization of $\frac{\boldsymbol{x^T L x}}{\boldsymbol{x^T x}}$
      - The (standard) Rayleigh quotient is scale invariant so limiting $x^{\mathrm{T}}x$ to any constant does not change its value
      - By the min-max theorem, $\lambda_{k-1}$ is minimal among all $\frac{x^{\mathrm{T}}Lx}{x^{\mathrm{T}}x}$ that are orthogonal to $\mu_k$
  - $x^{\mathrm{T}}\mathbf{1} = 0$
    - Automatically fulfilled by $\mu_{k-1}$
  - Ineffective: no longer ensures balance

    Both $\frac{[1\ 1\ {-1}\ \ {-1}\,]}{\|[1\ 1\ {-1}\ \ {-1}\,]\|}$ and $\frac{[1\ 1\ 1\ {-3}\,]}{\|[1\ 1\ 1\ {-3}\,]\|}$ fulfill the constraints

# Relaxed Rayleigh quotient version

- Eigenvalues

| $\lambda_1$ | $\lambda_2$ | $\lambda_3$ | $\lambda_4$ |
|---|---|---|---|
| 4.0000 | 3.0000 | 1.0000 | 0.0000 |

- Eigenvectors

| $\mu_1$ | $\mu_2$ | $\mu_3$ | $\mu_4$ |
|---|---|---|---|
| 0.8660 | 0.0000 | 0.0000 | -0.5000 |
| -0.2887 | 0.7071 | -0.4082 | -0.5000 |
| -0.2887 | -0.7071 | -0.4082 | -0.5000 |
| -0.2887 | 0.0000 | 0.8165 | -0.5000 |

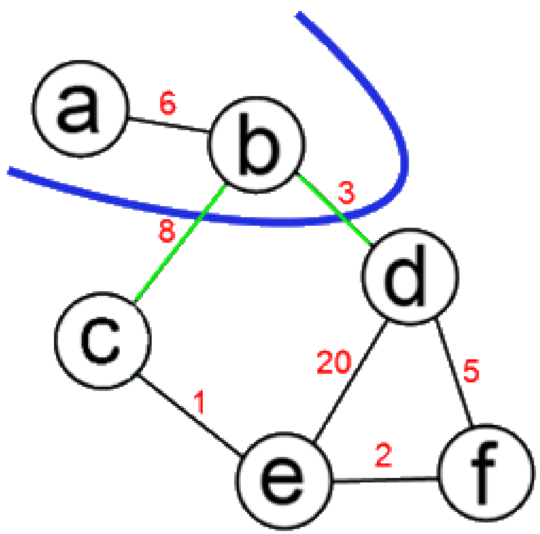
- As expected $\mu_4 = b\mathbf{1}$ $(b = -0.5)$ gives the trivial solution
- As expected $\lambda_3 \leq 2$, the optimal solution under constraint, since $\lambda_3$ is minimal among all $\frac{x^{\mathrm{T}}Lx}{x^{\mathrm{T}}x}$ for $x$ orthogonal to $\mu_4$

# Introducing weights into problems

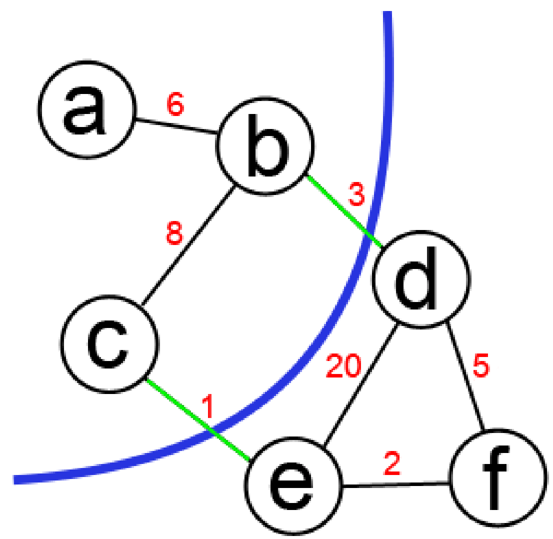
- Unweighted (undirected) graphs
  - Unbalanced version
    - (Unweighted) Minimum Cut Problem
  - Balanced version
    - Minimum Bisection Problem (NP-hard)
- Weighted (undirected) graphs
  - Unbalanced version
    - (Weighted) Minimum Cut Problem $O(|V||E|)$
  - Balanced versions
    - Ratio Cut Problem (NP-hard)
    - Graph Partitioning Problem (NP-hard)

# (Weighted) Minimum Cut Problem

- Given edge weight matrix $W = (w_{ij})$, the minimum cut of an undirected graph $G = (V, E)$ is a partition of $V$ into two groups $S$ and $\bar{S}$ such that $\text{cut}(S, \bar{S}) = \sum_{i \in S, j \in \bar{S}} w_{ij}$ is minimized




$\text{cut}(A, B) = 11$




$\text{cut}(A, B) = 4$

# (Weighted) Minimum Cut Problem

- Given edge weight matrix $W = (w_{ij})$, the minimum cut of an undirected graph $G = (V, E)$ is a partition of $V$ into two groups $S$ and $\bar{S}$ such that $\mathrm{cut}(S, \bar{S}) = \sum_{i \in S, j \in \bar{S}} w_{ij}$ is minimized
  - Ford-Fulkerson algorithm
  - Edmonds-Karp algorithm
  - Current best algorithm runs in $O(|V||E|)$ time
    - No point in using spectral clustering
    - Just as an example try anyway
    - First, define the graph Laplacian with edge weights

# Graph Laplacian with edge weights

- To add weight to the Laplacian
  - Adjacency matrix $A \Longrightarrow$ weight matrix $W$
  - Degree matrix $D \Longrightarrow$ weighted degree $D'$
- Laplacian $L = D - A$ becomes $L = D' - W$
- Given edge weights $W = \left(w_{ij}\right)_{m\times m}$, for any vector $x \in \mathbb{R}^m$,

$$x^{\mathrm{T}}(D' - W)x = \frac{1}{2}\sum_{1\le i,j\le m} w_{ij}\left(x_i - x_j\right)^2$$

(Proof same as for $x^{\mathrm{T}}(D - A)x = \frac{1}{2}\sum_{1\le i,j\le m} a_{ij}\left(x_i - x_j\right)^2$)

# Graph Laplacian with edge weights

- To add weight to the Laplacian
  - Adjacency matrix $A \Longrightarrow$ weight matrix $W$
  - Degree matrix $D \Longrightarrow$ weighted degree $D'$
- Laplacian $L = D - A$ becomes $L = D' - W$
- Suppose $x$ is a vector of only the values +1 and -1. Then,

$$x^{\mathrm{T}}(D' - W)x = \frac{1}{2}\sum\nolimits_{1\le i,j\le m} w_{ij}\left(x_i - x_j\right)^2$$

$$= \frac{1}{2}\sum\nolimits_{1\le i,j\le m} w_{ij}\left(x_i - x_j\right)^2 = 4\sum\nolimits_{1\le i<j\le m, x_i\ne x_j} w_{ij}$$

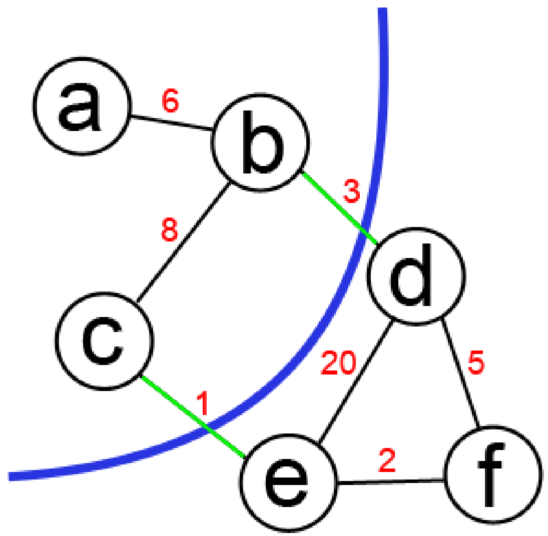
$$= 4\,\mathrm{cut}(A, B)$$

# Constrained optimization problem

- Minimize $x^{\mathrm{T}}Lx$ where $L = D' - W$ subject to $x_i \in \{1, -1\}$

- Example of cuts with $x^T Lx$ and Rayleigh quotient

| Group 1 | Group 2 | $x^T Lx$ | $\frac{x^T Lx}{x^T x}$ |
|---|---|---|---|
| A | B C D E F | 24 | 4.00 |
| A B C D E | F | 28 | 4.67 |
| A B | C D E F | 44 | 7.33 |
| A B C E | D F | 100 | 16.67 |
| A B C D | E F | 104 | 17.33 |
| A B C | D E F | 16 | 2.67 |
| A B D | C E F | 132 | 22.00 |




$\mathrm{cut}(A, B) = 4$

# Relaxed Rayleigh quotient version

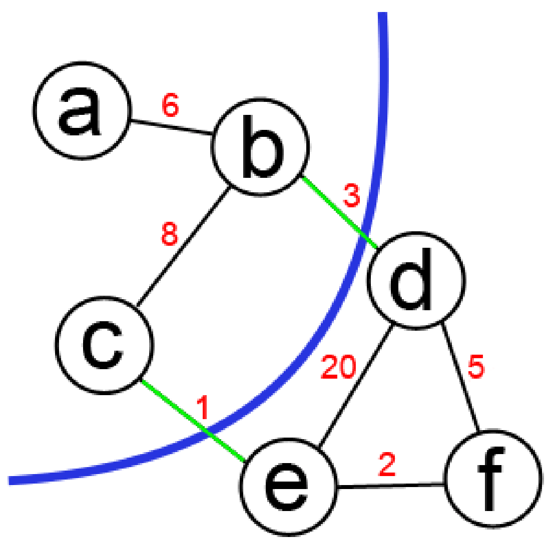
- Minimize $x^{\mathrm{T}}Lx$ where $L = D' - W$ subject to $x^{\mathrm{T}}x = 1$

Eigenvalues

| $\lambda_1$ | $\lambda_2$ | $\lambda_3$ | $\lambda_4$ | $\lambda_5$ | $\lambda_6$ |
|---|---|---|---|---|---|
| 46.04 | 23.36 | 11.07 | 7.28 | **2.25** | 0.00 |

Eigenvectors

| $\mu_1$ | $\mu_2$ | $\mu_3$ | $\mu_4$ | $\mu_5$ | $\mu_6$ |
|---|---|---|---|---|---|
| -0.0136 | -0.2879 | -0.0224 | -0.6854 | -0.5291 | -0.4082 |
| 0.0907 | 0.8331 | 0.0189 | 0.1460 | -0.3306 | -0.4082 |
| -0.0371 | -0.4557 | 0.1779 | 0.6912 | -0.3390 | -0.4082 |
| -0.7519 | 0.0242 | -0.3924 | 0.0007 | 0.3368 | -0.4082 |
| 0.6488 | -0.1212 | -0.5194 | 0.0226 | 0.3570 | -0.4082 |
| 0.0631 | 0.0074 | 0.7374 | -0.1750 | 0.5049 | -0.4082 |




$\mathrm{cut}(A, B) = 4$

# Ratio Cut Problem

- Given edge weight matrix $W = (w_{ij})$, the minimum ratio cut of an undirected graph $G = (V, E)$ is a partition of $V$ into two groups $S$ and $\bar{S}$ such that

$$\text{ratio}(S, \bar{S}) = \text{cut}(S, \bar{S}) \left( \frac{1}{|S|} + \frac{1}{|\bar{S}|} \right)$$

  is minimized, where $\text{cut}(S, \bar{S}) = \sum_{i \in S, j \in \bar{S}} w_{ij}$

- Original paper defined $\text{ratio}(S, \bar{S}) = \text{cut}(S, \bar{S}) / |S||\bar{S}|$

$$= \frac{1}{|V|} \text{cut}(S, \bar{S}) \left( \frac{1}{|S|} + \frac{1}{|\bar{S}|} \right)$$

# Ratio Cut

- Represent a partition $S, \bar{S}$ of $V$ with $x \in \mathbb{R}^n$, where

$$x_i = \begin{cases} \sqrt{\frac{|S|}{|\bar{S}|}} & \text{if } i \in S \\ -\sqrt{\frac{|\bar{S}|}{|S|}} & \text{if } i \in \bar{S} \end{cases}$$

- Then, $x^{\mathrm{T}}x = |S|\frac{|\bar{S}|}{|S|} + |\bar{S}|\frac{|S|}{|\bar{S}|} = |V| = \text{const}$

- $\sum_i x_i = \sum_{i \in S}\sqrt{\frac{|\bar{S}|}{|S|}} - \sum_{v_i \in \bar{S}}\sqrt{\frac{|S|}{|\bar{S}|}} = |S|\sqrt{\frac{|\bar{S}|}{|S|}} - |\bar{S}|\sqrt{\frac{|S|}{|\bar{S}|}} = 0$

  $\Rightarrow x \perp \mathbf{1}$ (in fact, it can be shown that $x \perp b\mathbf{1}$ for any $b$)

- For the unnormalized weighted Laplacian $L = D' - W$

$$x^{\mathrm{T}}Lx = |V|\mathrm{cut}(S, \bar{S})\left(\frac{1}{|S|} + \frac{1}{|\bar{S}|}\right) = |V|\mathrm{ratio}(S, \bar{S})$$

# Proof for $x^{\mathrm{T}}Lx = |V|\mathrm{ratio}(S,\bar{S})$

- $x^{\mathrm{T}}Lx = \frac{1}{2}\sum_{1\le i,j\le m} w_{ij}\left(x_i - x_j\right)^2$

$$= \frac{1}{2}\sum_{i\in S, j\in\bar{S}} w_{ij}\left(\sqrt{\frac{|S|}{|\bar{S}|}} + \sqrt{\frac{|\bar{S}|}{|S|}}\right)^2 + \frac{1}{2}\sum_{i\in S, j\in\bar{S}} w_{ij}\left(-\sqrt{\frac{|S|}{|\bar{S}|}} - \sqrt{\frac{|\bar{S}|}{|S|}}\right)^2$$

$$= \sum_{i\in S, j\in\bar{S}} w_{ij}\left(\frac{|S|}{|\bar{S}|} + \frac{|\bar{S}|}{|S|} + 2\right) = \mathrm{cut}(S,\bar{S})\left(\frac{|S|}{|\bar{S}|} + \frac{|\bar{S}|}{|S|} + 2\right)$$

$$= \mathrm{cut}(S,\bar{S})\left(\frac{|S|}{|\bar{S}|} + \frac{|\bar{S}|}{|S|} + \frac{|S|}{|S|} + \frac{|\bar{S}|}{|\bar{S}|}\right)$$

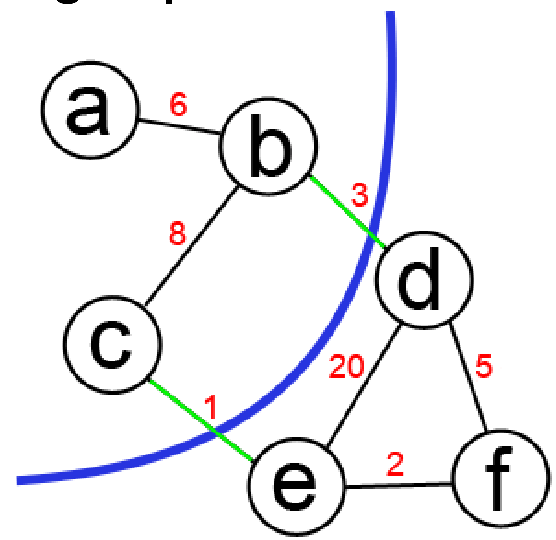
$$= \mathrm{cut}(S,\bar{S})\left(\frac{|S| + |\bar{S}|}{|\bar{S}|} + \frac{|S| + |\bar{S}|}{|S|}\right)$$

$$= (|S| + |\bar{S}|)\mathrm{cut}(S,\bar{S})\left(\frac{1}{|\bar{S}|} + \frac{1}{|S|}\right) = |V|\mathrm{cut}(S,\bar{S})\left(\frac{1}{|\bar{S}|} + \frac{1}{|S|}\right)$$

# Constrained optimization problem

- Minimize $x^{\mathrm{T}}Lx$ where $L = D' - W$ subject to $x_i \in \{1, -1\}$ and $x^{\mathrm{T}}\mathbf{1} = 0$
  - $x_i \in \{1, -1\}$ and $x^{\mathrm{T}}\mathbf{1} = 0$ enforce balance
  - However, problem is NP-hard
- Example of cuts with $x^T Lx$ and Rayleigh quotient

| Group 1 | Group 2 | $x^T Lx$ | $\frac{x^T Lx}{x^T x}$ |
|---|---|---|---|
| A | B C D E F | 24 | 4.00 |
| A B C D E | F | 28 | 4.67 |
| A B | C D E F | 44 | 7.33 |
| A B C E | D F | 100 | 16.67 |
| A B C D | E F | 104 | 17.33 |
| **A B C** | **D E F** | **16** | **2.67** |
| A B D | C E F | 132 | 22.00 |




$\mathrm{cut}(A, B) = 4$

# Relaxed Rayleigh quotient version

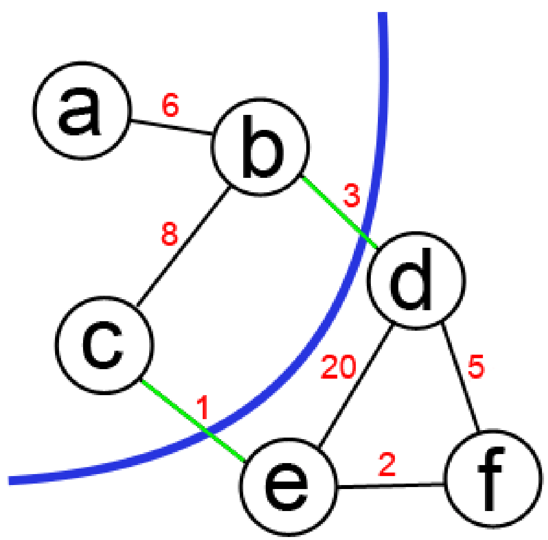
- Minimize $x^{\mathrm{T}} L x$ where $L = D' - W$ subject to $x^{\mathrm{T}} x = 1$ and $x^{\mathrm{T}} \mathbf{1} = 0$
  - Balance no longer enforced

Eigenvalues

| $\lambda_1$ | $\lambda_2$ | $\lambda_3$ | $\lambda_4$ | $\lambda_5$ | $\lambda_6$ |
|---|---|---|---|---|---|
| 46.04 | 23.36 | 11.07 | 7.28 | **2.25** | 0.00 |

Eigenvectors

| $\mu_1$ | $\mu_2$ | $\mu_3$ | $\mu_4$ | $\mu_5$ | $\mu_6$ |
|---|---|---|---|---|---|
| -0.0136 | -0.2879 | -0.0224 | -0.6854 | -0.5291 | -0.4082 |
| 0.0907 | 0.8331 | 0.0189 | 0.1460 | -0.3306 | -0.4082 |
| -0.0371 | -0.4557 | 0.1779 | 0.6912 | -0.3390 | -0.4082 |
| -0.7519 | 0.0242 | -0.3924 | 0.0007 | 0.3368 | -0.4082 |
| 0.6488 | -0.1212 | -0.5194 | 0.0226 | 0.3570 | -0.4082 |
| 0.0631 | 0.0074 | 0.7374 | -0.1750 | 0.5049 | -0.4082 |




$\mathrm{cut}(A, B) = 4$

# Relaxed Rayleigh quotient version

Eigenvalues

| $\lambda_1$ | $\lambda_2$ | $\lambda_3$ | $\lambda_4$ | $\lambda_5$ | $\lambda_6$ |
|---|---|---|---|---|---|
| 46.04 | 23.36 | 11.07 | 7.28 | **2.25** | 0.00 |

Eigenvectors

| $\mu_1$ | $\mu_2$ | $\mu_3$ | $\mu_4$ | $\mu_5$ | $\mu_6$ |
|---|---|---|---|---|---|
| -0.0136 | -0.2879 | -0.0224 | -0.6854 | -0.5291 | -0.4082 |
| 0.0907 | 0.8331 | 0.0189 | 0.1460 | -0.3306 | -0.4082 |
| -0.0371 | -0.4557 | 0.1779 | 0.6912 | -0.3390 | -0.4082 |
| -0.7519 | 0.0242 | -0.3924 | 0.0007 | 0.3368 | -0.4082 |
| 0.6488 | -0.1212 | -0.5194 | 0.0226 | 0.3570 | -0.4082 |
| 0.0631 | 0.0074 | 0.7374 | -0.1750 | 0.5049 | -0.4082 |

The eigenvalue system is exactly the same as in (Weighted) Minimum Cut – only the optimal solution is different

- As expected $\mu_6 = b\mathbf{1}$ $(b = -0.4082)$ gives the trivial solution
- As expected $\lambda_5 \leq 2.67$, the optimal solution under constraint, since $\lambda_5$ is minimal among all $\frac{x^{\mathrm{T}}Lx}{x^{\mathrm{T}}x}$ for $x$ orthogonal to $\mu_6$

# Comparison of problems

- Unweighted problem ($L = D - A$)
  - Minimum Cut
  - Add balance ⇒ Minimum Bisection
- Weighted problems ($L = D' - W$)
  - (Weighted) Minimum Cut
  - Add balance ⇒ Ratio Cut

- The version of the problem with $x\mathbf{1} = 0$ balance requirement can better exploit the fact that $\mu_{k-1} \perp \mu_k$ where $\mu_k = \mathbf{1}$ to claim optimality
- However note that even with $x^{\mathrm{T}}\mathbf{1} = 0$, the balance requirement is not ensured

# More constraint for balance

- So far, no attempt has been made to maintain the balance of the partition besides $x^{\mathrm{T}}x = 1$ and $x^{\mathrm{T}}\mathbf{1} = 0$, both of which are fulfilled automatically for a eigenvalue system
- Further constraints can be added to the eigenvalue system
  - However, the resultant eigenvalue system will no longer be standard
  - Demonstrate with Graph Partitioning Problem in Part 3