
CS 267

Lecture 18: Graph Partitioning

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[slides from James Demmel and John Gilbert]

<https://sites.google.com/lbl.gov/cs267-spr2019/>

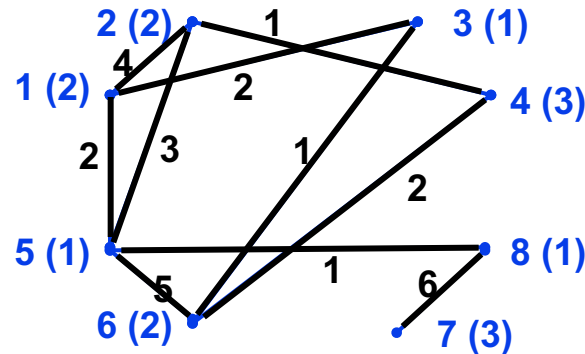
Outline of Graph Partitioning Lecture

- Review definition of Graph Partitioning problem
- Overview of heuristics
- Partitioning with Nodal Coordinates
 - Ex: In finite element models, node at point in (x,y) or (x,y,z) space
- Partitioning without Nodal Coordinates
 - Ex: In model of WWW, nodes are web pages
- Multilevel Acceleration
 - **BIG IDEA**, appears often in scientific computing
- Available Implementations
- Beyond Graph Partitioning: Hypergraphs

Definition of Graph Partitioning

- Given a graph $G = (N, E, W_N, W_E)$

- N = nodes (or vertices),
- W_N = node weights
- E = edges
- W_E = edge weights

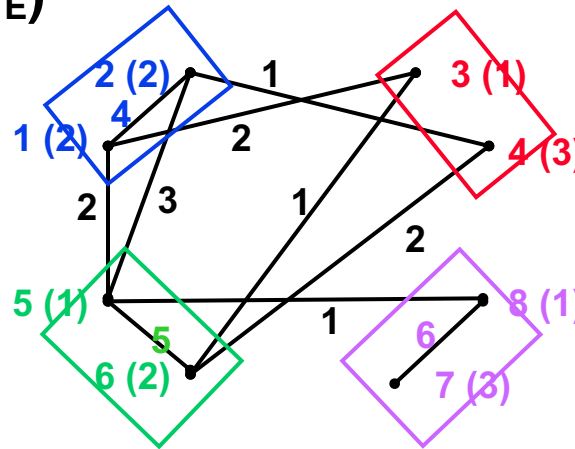


- Ex: $N = \{\text{tasks}\}$, $W_N = \{\text{task costs}\}$, edge (j,k) in E means task j sends $W_E(j,k)$ words to task k
- Choose a partition $N = N_1 \cup N_2 \cup \dots \cup N_p$ such that
 - The sum of the node weights in each N_j is “about the same”
 - The sum of all edge weights of edges connecting all different pairs N_j and N_k is minimized
- Ex: balance the work load, while minimizing communication
- Special case of $N = N_1 \cup N_2$: Graph Bisection

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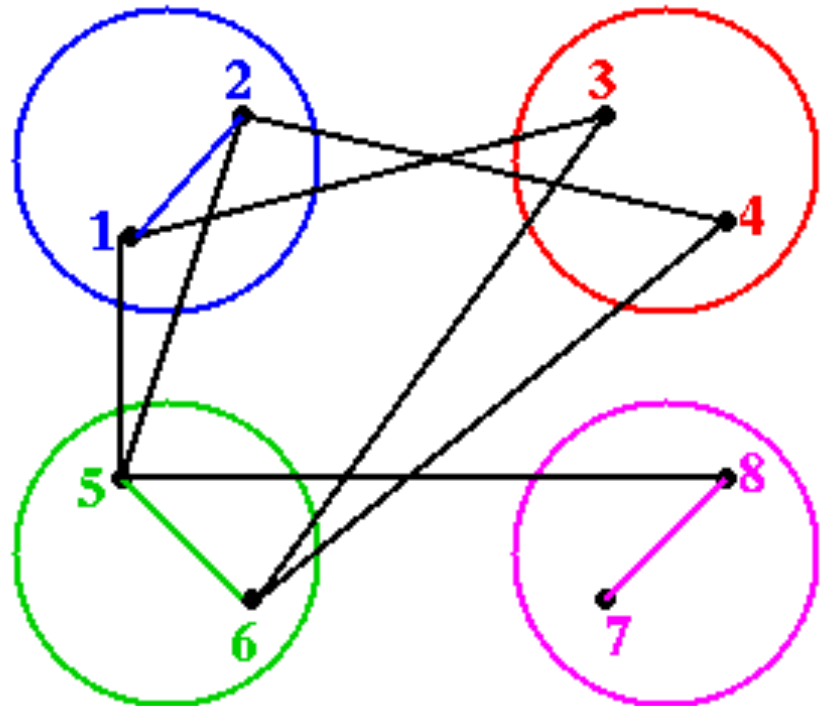
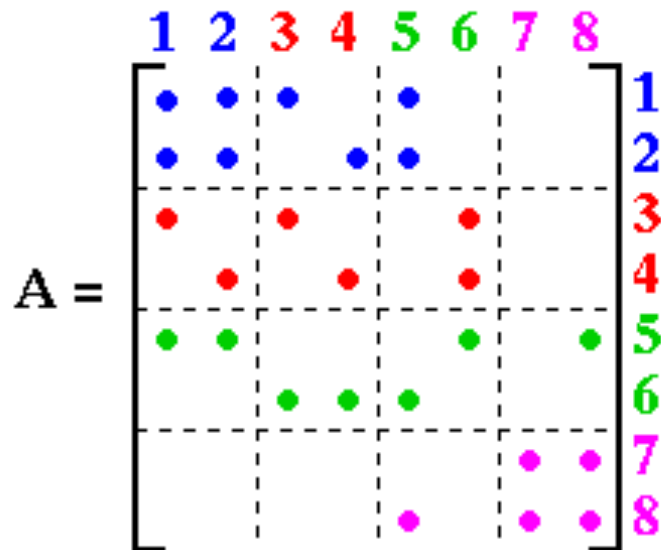
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 - The sum of the node weights in each N_j is “about the same”
 - The sum of all edge weights of edges connecting all different pairs N_j and N_k is minimized (shown in black)
- Ex: balance the work load, while minimizing communication
- Special case of $N = N_1 \cup N_2$: Graph Bisection

Some Applications

- Telephone network design
 - Original application, algorithm due to Kernighan
- Load Balancing while Minimizing Communication
- Sparse Matrix times Vector Multiplication (SpMV)
 - Solving PDEs
 - $N = \{1, \dots, n\}$, $(j, k) \in E$ if $A(j, k)$ nonzero,
 - $W_N(j) = \text{\#nonzeros in row } j$, $W_E(j, k) = 1$
- VLSI Layout
 - $N = \{\text{units on chip}\}$, $E = \{\text{wires}\}$, $W_E(j, k) = \text{wire length}$
- Sparse Gaussian Elimination
 - Used to reorder rows and columns to increase parallelism, and to decrease “fill-in”
- Data mining and clustering
- Physical Mapping of DNA
- Image Segmentation

Sparse Matrix Vector Multiplication $y = y + A * x$

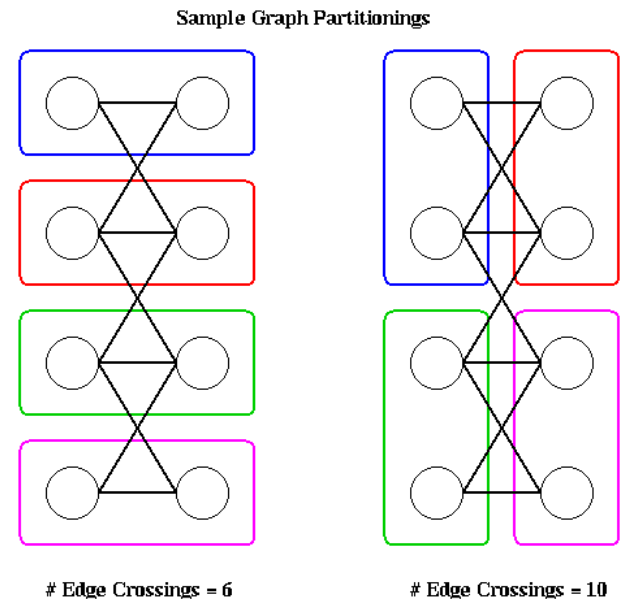
Partitioning a Sparse Symmetric Matrix



```
... declare A_local, A_remote(1:num_procs), x_local, x_remote, y_local
y_local = y_local + A_local * x_local
for all procs P that need part of x_local
    send(needed part of x_local, P)
for all procs P owning needed part of x_remote
    receive(x_remote, P)
    y_local = y_local + A_remote(P)*x_remote
```

Cost of Graph Partitioning

- Many possible partitionings to search
- Just to divide in 2 parts there are:
 $n \text{ choose } n/2 = n!/((n/2)!)^2 \sim (2/(n\pi))^{1/2} * 2^n$ possibilities



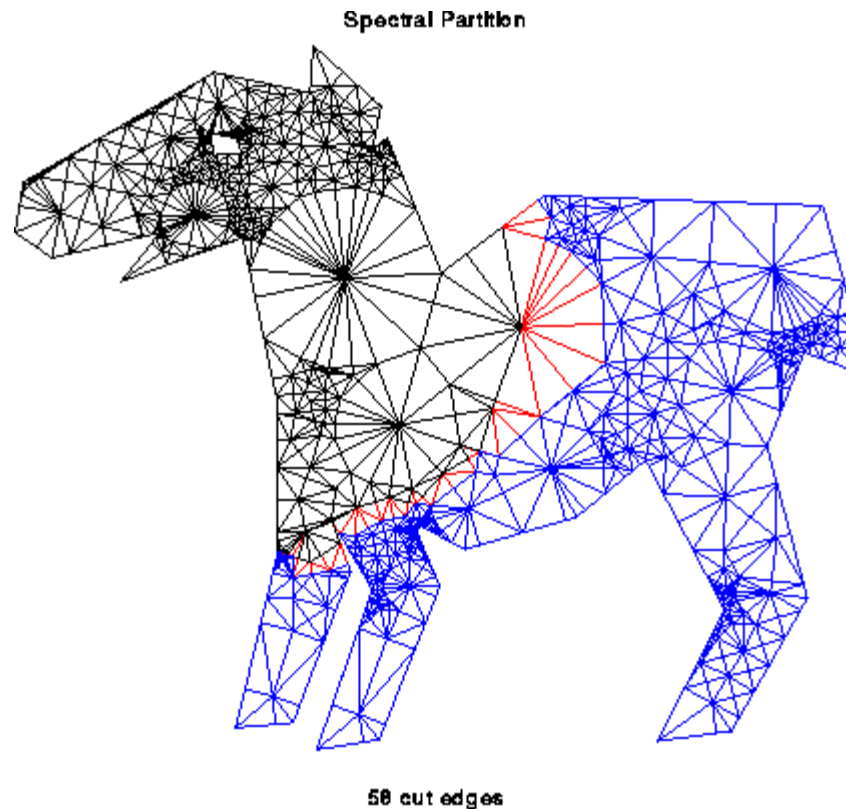
- Choosing optimal partitioning is NP-complete
 - (NP-complete = we can prove it is as hard as other well-known hard problems in a class Nondeterministic Polynomial time)
 - Only known exact algorithms have cost = exponential(n)
- We need good heuristics

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First Heuristic: Repeated Graph Bisection

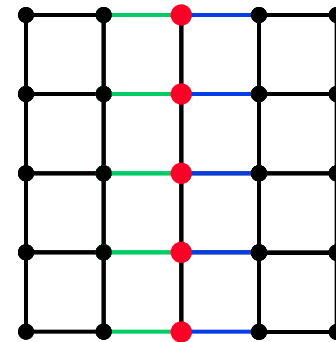
- To partition N into 2^k parts
 - bisect graph recursively k times
- Henceforth discuss mostly graph bisection



Edge Separators vs. Vertex Separators

- **Edge Separator**: E_s (subset of E) separates G if removing E_s from E leaves two \sim equal-sized, disconnected components of N : N_1 and N_2
- **Vertex Separator**: N_s (subset of N) separates G if removing N_s and all incident edges leaves two \sim equal-sized, disconnected components of N : N_1 and N_2

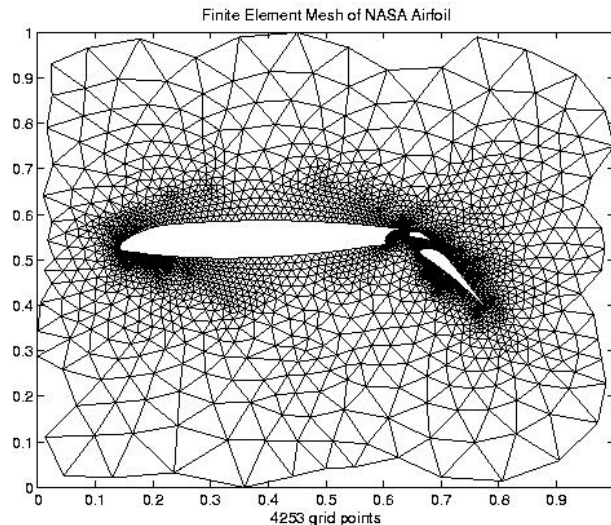
$G = (N, E)$, Nodes N and Edges E
 E_s = **green edges** or **blue edges**
 N_s = **red vertices**



- Making an N_s from an E_s : pick one endpoint of each edge in E_s
 - $|N_s| \leq |E_s|$
- Making an E_s from an N_s : pick all edges incident on N_s
 - $|E_s| \leq d * |N_s|$ where d is the maximum degree of the graph
- We will find Edge or Vertex Separators, as convenient

Overview of Bisection Heuristics

- Partitioning with Nodal Coordinates
 - Each node has x,y,z coordinates → partition space



- Partitioning without Nodal Coordinates
 - E.g., Sparse matrix of Web documents
 - $A(j,k) = \# \text{ times keyword } j \text{ appears in URL } k$
- Multilevel acceleration **(BIG IDEA)**
 - Approximate problem by “coarse graph,” do so recursively

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Nodal Coordinates: How Well Can We Do?

- A planar graph can be drawn in plane without edge crossings
- Ex: $m \times m$ grid of m^2 nodes: \exists vertex separator N_s with $|N_s| = m = |N|^{1/2}$ (see earlier slide for $m=5$)
- *Theorem* (Tarjan, Lipton, 1979): If G is planar, $\exists N_s$ such that
 - $N = N_1 \cup N_s \cup N_2$ is a partition,
 - $|N_1| \leq 2/3 |N|$ and $|N_2| \leq 2/3 |N|$
 - $|N_s| \leq (8 * |N|)^{1/2}$
- Theorem motivates intuition of following algorithms

Nodal Coordinates: Inertial Partitioning

- For a graph in 2D, choose line with half the nodes on one side and half on the other
 - In 3D, choose a plane, but consider 2D for simplicity
- Choose a line L , and then choose a line L^\perp perpendicular to it, with half the nodes on either side

1. Choose a line L through the points

L given by $a*(x-\bar{x})+b*(y-\bar{y})=0$,

with $a^2+b^2=1$; (a,b) is unit vector \perp to L

2. Project each point to the line

For each $n_j = (x_j, y_j)$, compute coordinate

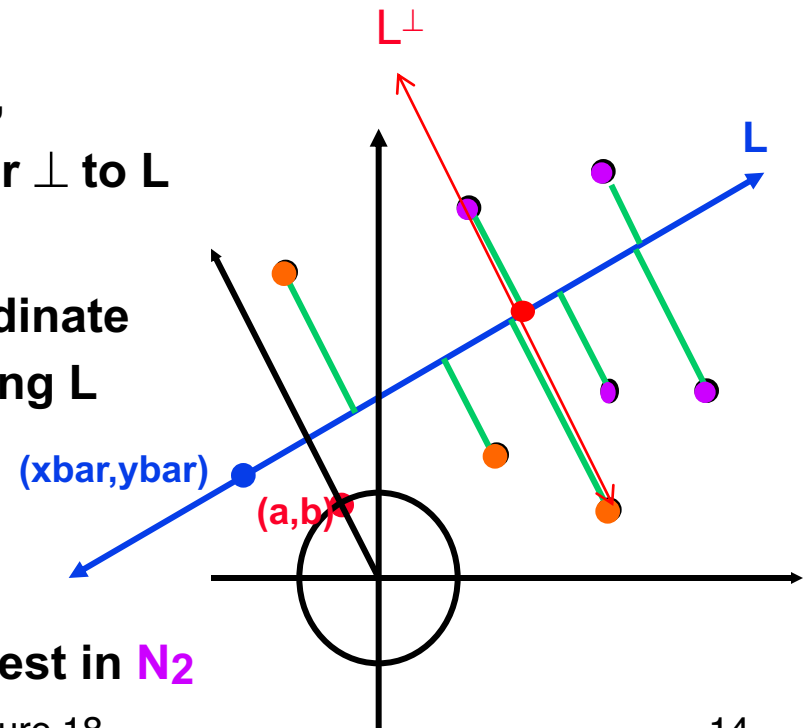
$S_j = -b*(x_j-\bar{x}) + a*(y_j-\bar{y})$ along L

3. Compute the median

Let $S_{\text{bar}} = \text{median}(S_1, \dots, S_n)$

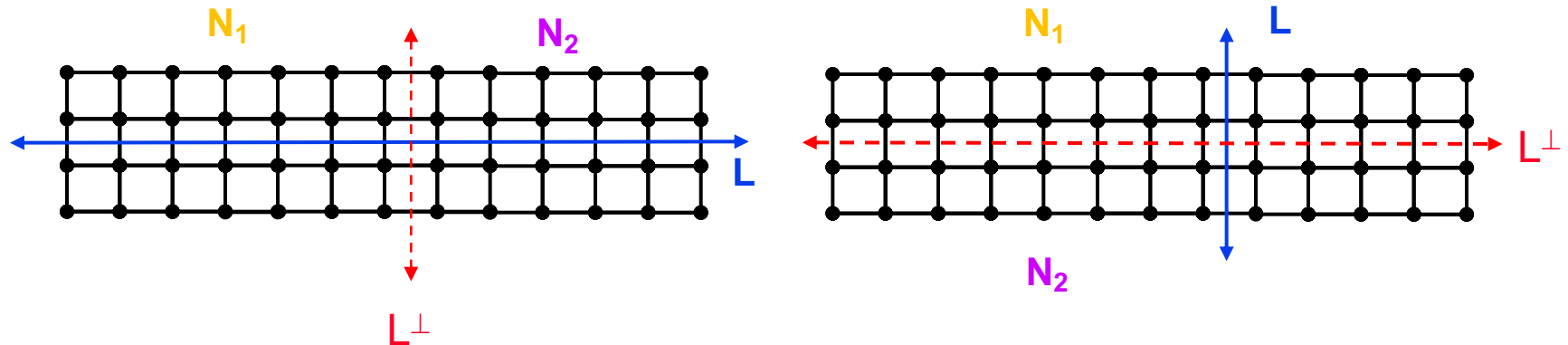
4. Use median to partition the nodes

Let nodes with $S_j < S_{\text{bar}}$ be in N_1 , rest in N_2



Inertial Partitioning: Choosing L

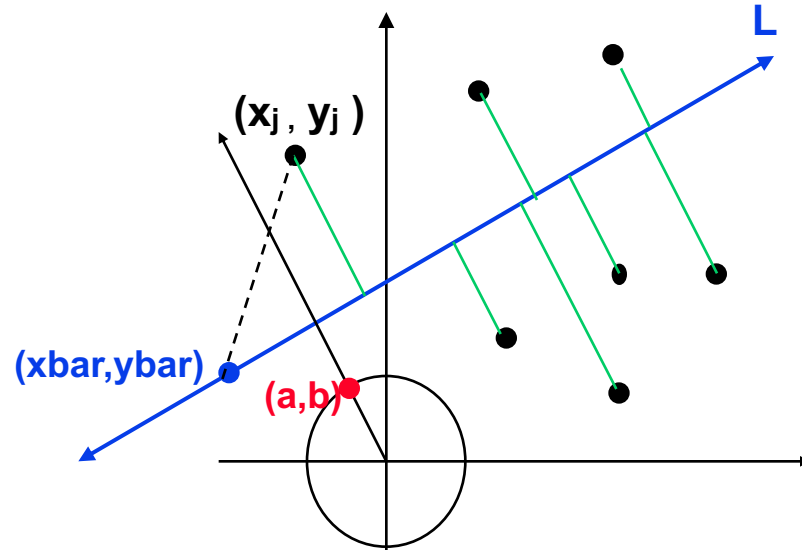
- Clearly prefer L, L^\perp on left below



- Mathematically, choose L to be a **total least squares fit of the nodes**
 - Minimize sum of squares of distances to L (green lines on last slide)
 - Equivalent to choosing L as axis of rotation that minimizes the moment of inertia of nodes (unit weights) - source of name

Inertial Partitioning: choosing L (continued)

(a,b) is unit vector
perpendicular to L



\sum_j (length of j-th green line)²

$$= \sum_j [(x_j - \bar{x})^2 + (y_j - \bar{y})^2 - (-b(x_j - \bar{x}) + a(y_j - \bar{y}))^2]$$

... **Pythagorean Theorem**

$$= a^2 \sum_j (x_j - \bar{x})^2 + 2ab \sum_j (x_j - \bar{x})(y_j - \bar{y}) + b^2 \sum_j (y_j - \bar{y})^2$$

$$= a^2 * X1 + 2ab * X2 + b^2 * X3$$

$$= [a \ b] * \begin{bmatrix} X1 & X2 \\ X2 & X3 \end{bmatrix} * \begin{bmatrix} a \\ b \end{bmatrix}$$

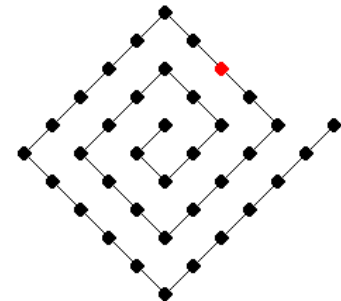
Minimized by choosing

$(\bar{x}, \bar{y}) = (\sum_j x_j, \sum_j y_j) / n = \text{center of mass}$

(a,b) = eigenvector of smallest eigenvalue of $\begin{bmatrix} X1 & X2 \\ X2 & X3 \end{bmatrix}$

Nodal Coordinates: Summary

- Other variations on these algorithms
- Algorithms are efficient
- Rely on graphs having nodes connected (mostly) to “nearest neighbors” in space
 - algorithm does not depend on where actual edges are!
- Common when graph arises from physical model
- Ignores edges, but can be used as good starting guess for subsequent partitioners that do examine edges
- Can do poorly if graph connectivity is not spatial:
- Details at
 - www.cs.berkeley.edu/~demmell/cs267/lecture18/lec
 - www.cs.ucsb.edu/~gilbert
 - www-bcf.usc.edu/~shanghua/



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Coordinate-Free: Kernighan/Lin

- Take a initial partition and iteratively improve it
 - Kernighan/Lin (1970), cost = $O(|N|^3)$ but easy to understand
 - Fiduccia/Mattheyses (1982), cost = $O(|E|)$, much better, but more complicated
- Given $G = (N, E, W_E)$ and a partitioning $N = A \cup B$, where $|A| = |B|$
 - $T = \text{cost}(A, B) = \sum \{W(e) \text{ where } e \text{ connects nodes in } A \text{ and } B\}$
 - Find subsets X of A and Y of B with $|X| = |Y|$
 - Consider swapping X and Y if it decreases cost:
 - $\text{newA} = (A - X) \cup Y$ and $\text{newB} = (B - Y) \cup X$
 - $\text{newT} = \text{cost}(\text{newA}, \text{newB}) < T = \text{cost}(A, B)$
- Need to compute newT efficiently for many possible X and Y , choose smallest (best)

Kernighan/Lin: Preliminary Definitions

- $T = \text{cost}(A, B)$, $\text{newT} = \text{cost}(\text{newA}, \text{newB})$
- Need an efficient formula for newT; will use
 - $E(a) = \text{external cost of } a \text{ in } A = \sum \{W(a,b) \text{ for } b \text{ in } B\}$
 - $I(a) = \text{internal cost of } a \text{ in } A = \sum \{W(a,a') \text{ for other } a' \text{ in } A\}$
 - $D(a) = \text{cost of } a \text{ in } A = E(a) - I(a)$
 - $E(b)$, $I(b)$ and $D(b)$ defined analogously for b in B
- Consider swapping $X = \{a\}$ and $Y = \{b\}$
 - $\text{newA} = (A - \{a\}) \cup \{b\}$, $\text{newB} = (B - \{b\}) \cup \{a\}$
- $\text{newT} = T - (D(a) + D(b) - 2 \cdot w(a,b)) \equiv T - \text{gain}(a,b)$
 - $\text{gain}(a,b)$ measures improvement gotten by swapping a and b
- Update formulas
 - $\text{newD}(a') = D(a') + 2 \cdot w(a',a) - 2 \cdot w(a',b)$ for $a' \text{ in } A, a' \neq a$
 - $\text{newD}(b') = D(b') + 2 \cdot w(b',b) - 2 \cdot w(b',a)$ for $b' \text{ in } B, b' \neq b$

Kernighan/Lin Algorithm

Compute $T = \text{cost}(A, B)$ for initial A, B

... cost = $O(|N|^2)$

Repeat

... One pass greedily computes $|N|/2$ possible X, Y to swap, picks best

Compute costs $D(n)$ for all n in N

... cost = $O(|N|^2)$

Unmark all nodes in N

... cost = $O(|N|)$

While there are unmarked nodes

... $|N|/2$ iterations

Find an unmarked pair (a, b) maximizing $\text{gain}(a, b)$

... cost = $O(|N|^2)$

Mark a and b (but do not swap them)

... cost = $O(1)$

Update $D(n)$ for all unmarked n ,

as though a and b had been swapped

... cost = $O(|N|)$

Endwhile

... At this point we have computed a sequence of pairs

... $(a_1, b_1), \dots, (a_k, b_k)$ and gains $\text{gain}(1), \dots, \text{gain}(k)$

... where $k = |N|/2$, numbered in the order in which we marked them

Pick m maximizing $\text{Gain} = \sum_{k=1}^m \text{gain}(k)$

... cost = $O(|N|)$

... Gain is reduction in cost from swapping (a_1, b_1) through (a_m, b_m)

If $\text{Gain} > 0$ then ... it is worth swapping

Update $\text{newA} = A - \{a_1, \dots, a_m\} \cup \{b_1, \dots, b_m\}$

... cost = $O(|N|)$

Update $\text{newB} = B - \{b_1, \dots, b_m\} \cup \{a_1, \dots, a_m\}$

... cost = $O(|N|)$

Update $T = T - \text{Gain}$

... cost = $O(1)$

endif

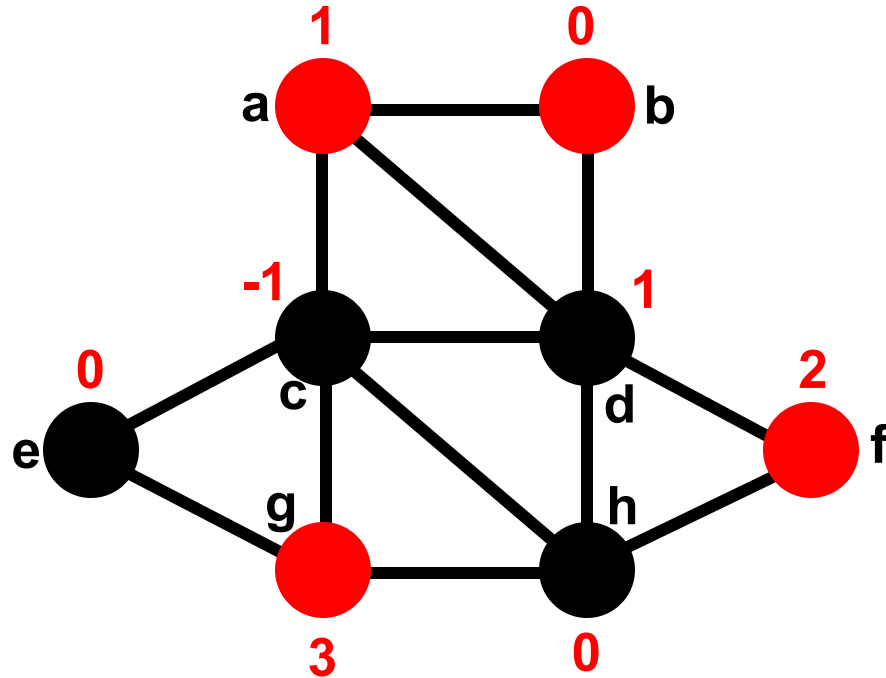
Until $\text{Gain} \leq 0$

Simplified Fiduccia-Mattheyses: Example (1)

Red nodes are in Part1;
black nodes are in Part2.

The initial partition into two parts is arbitrary. In this case it cuts 8 edges.

The initial node gains are shown in red.



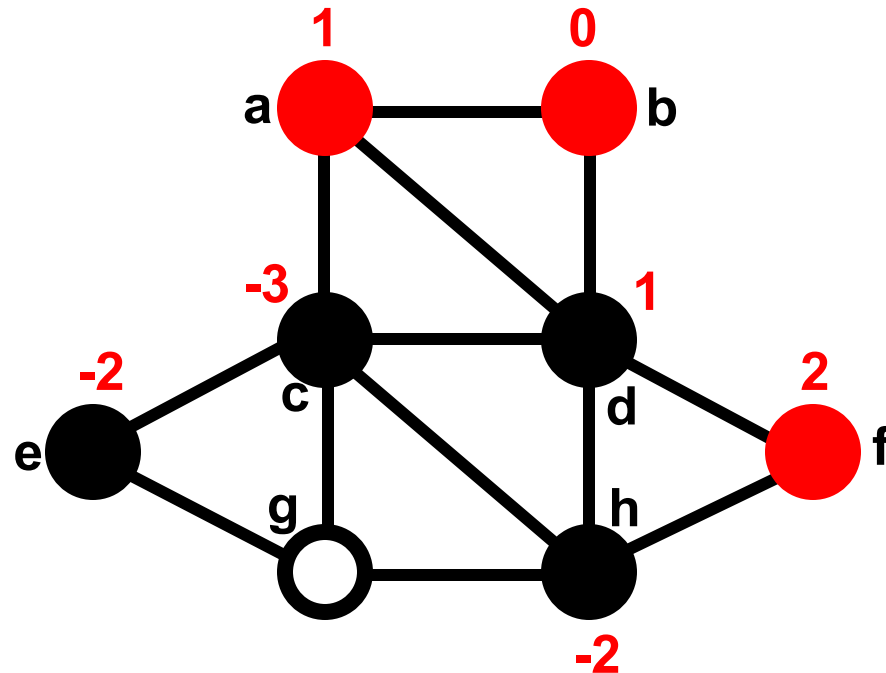
Nodes tentatively moved (and cut size after each pair):

none (8);

Simplified Fiduccia-Mattheyses: Example (2)

The node in Part1 with largest gain is g. We tentatively move it to Part2 and recompute the gains of its neighbors.

Tentatively moved nodes are hollow circles. After a node is tentatively moved its gain doesn't matter any more.



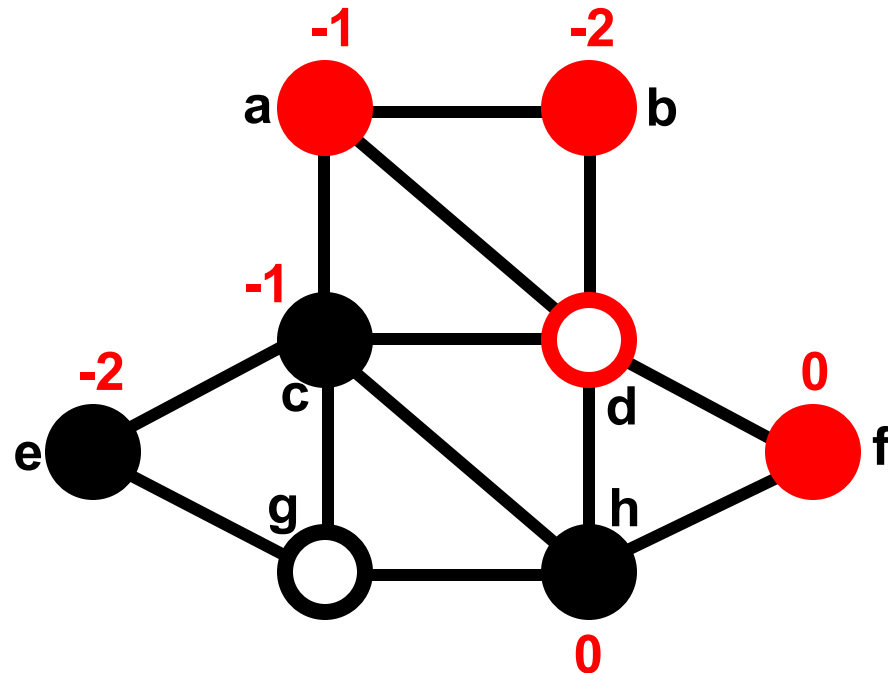
Nodes tentatively moved (and cut size after each pair):

none (8); g,

Simplified Fiduccia-Mattheyses: Example (3)

The node in Part2 with largest gain is d. We tentatively move it to Part1 and recompute the gains of its neighbors.

After this first tentative swap, the cut size is 4.

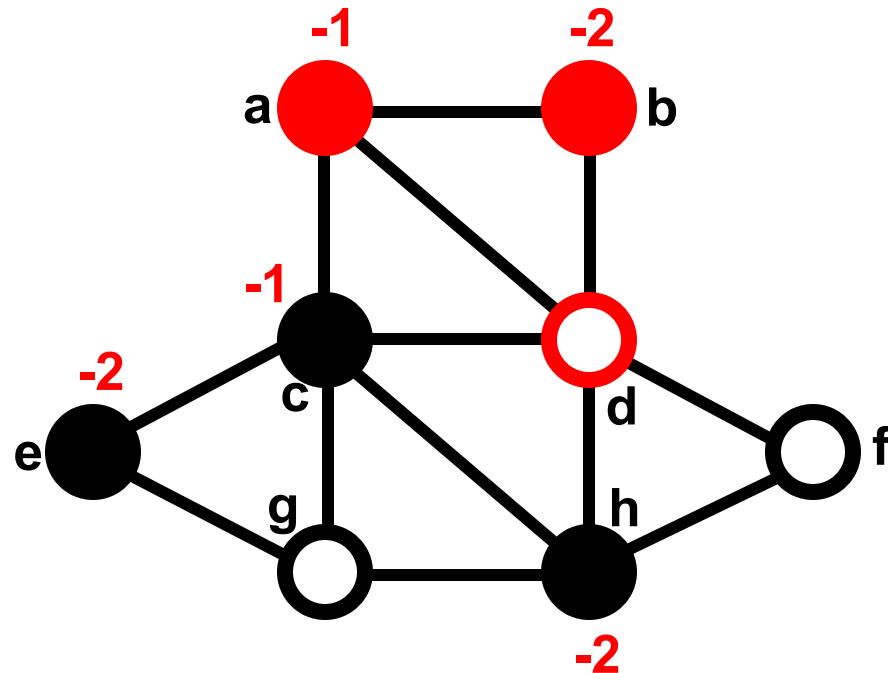


Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4);

Simplified Fiduccia-Mattheyses: Example (4)

The unmoved node in Part1 with largest gain is f. We tentatively move it to Part2 and recompute the gains of its neighbors.



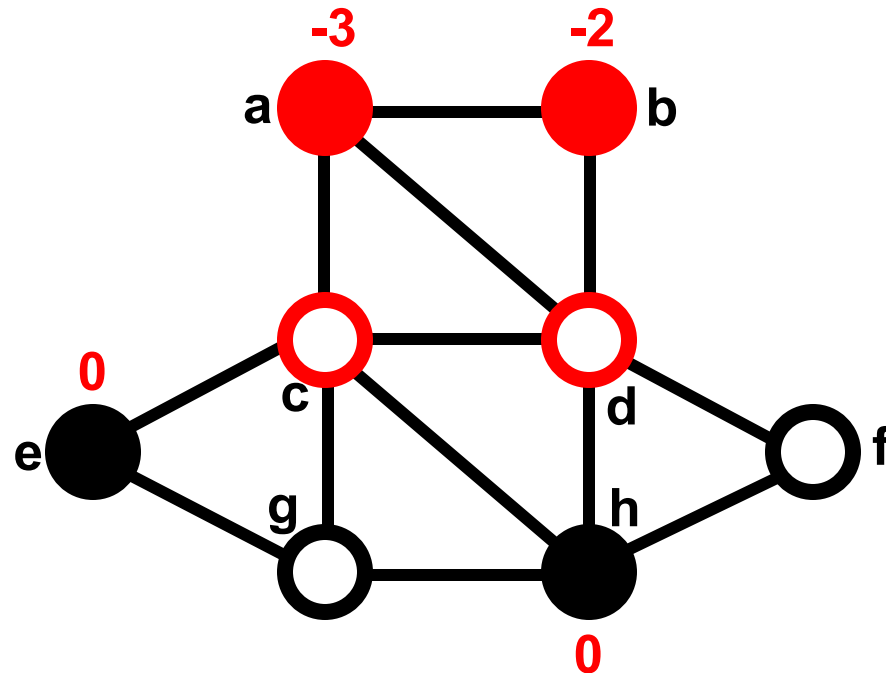
Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f

Simplified Fiduccia-Mattheyses: Example (5)

The unmoved node in Part2 with largest gain is c.
We tentatively move it to Part1 and recompute the gains of its neighbors.

After this tentative swap,
the cut size is 5.

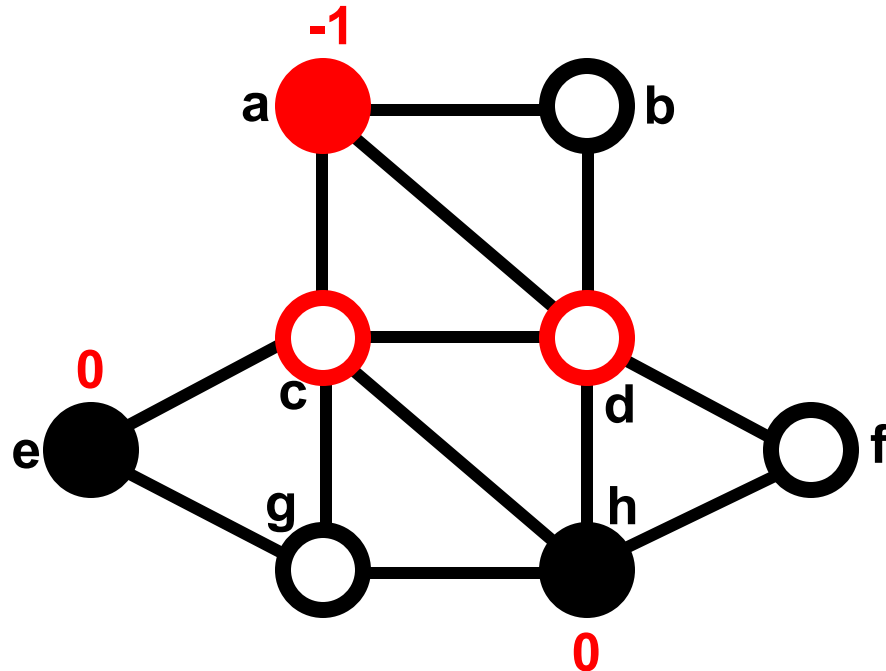


Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5);

Simplified Fiduccia-Mattheyses: Example (6)

The unmoved node in Part1 with largest gain is b.
We tentatively move it to Part2 and recompute the gains of its neighbors.



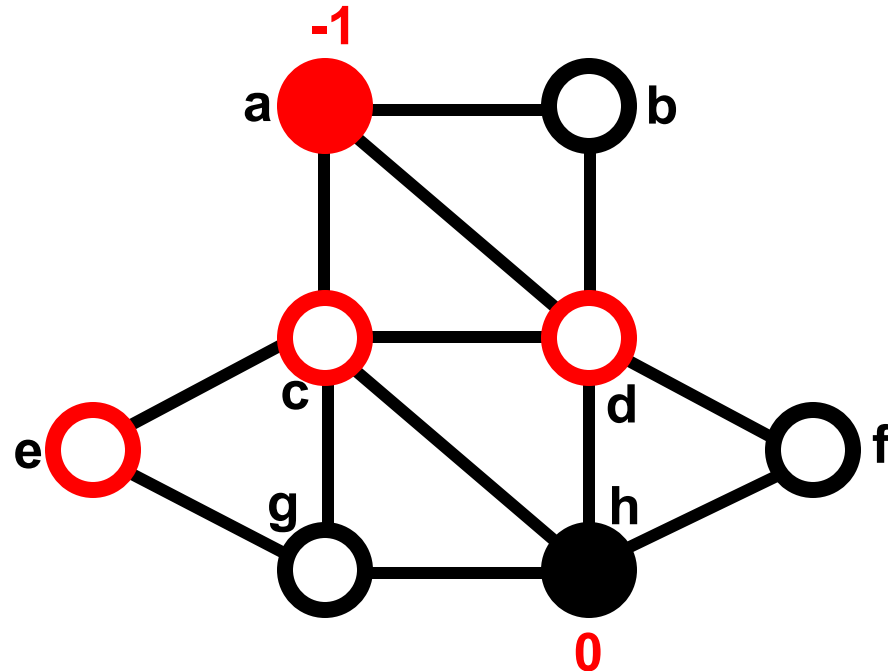
Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5); b

Simplified Fiduccia-Mattheyses: Example (7)

There is a tie for largest gain between the two unmoved nodes in Part2. We choose one (say e) and tentatively move it to Part1. It has no unmoved neighbors so no gains are recomputed.

After this tentative swap the cut size is 7.

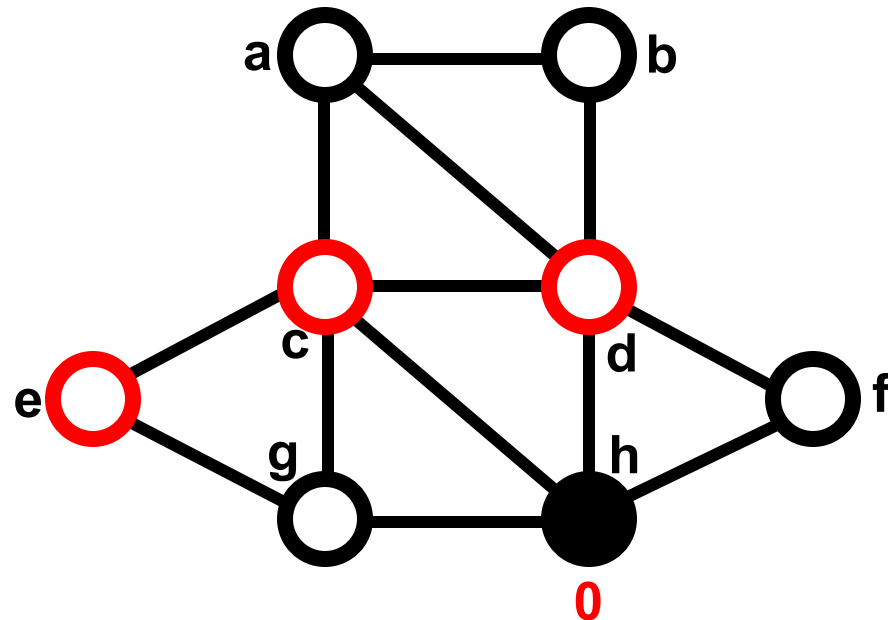


Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5); b, e (7);

Simplified Fiduccia-Mattheyses: Example (8)

The unmoved node in Part1 with the largest gain (the only one) is a. We tentatively move it to Part2. It has no unmoved neighbors so no gains are recomputed.



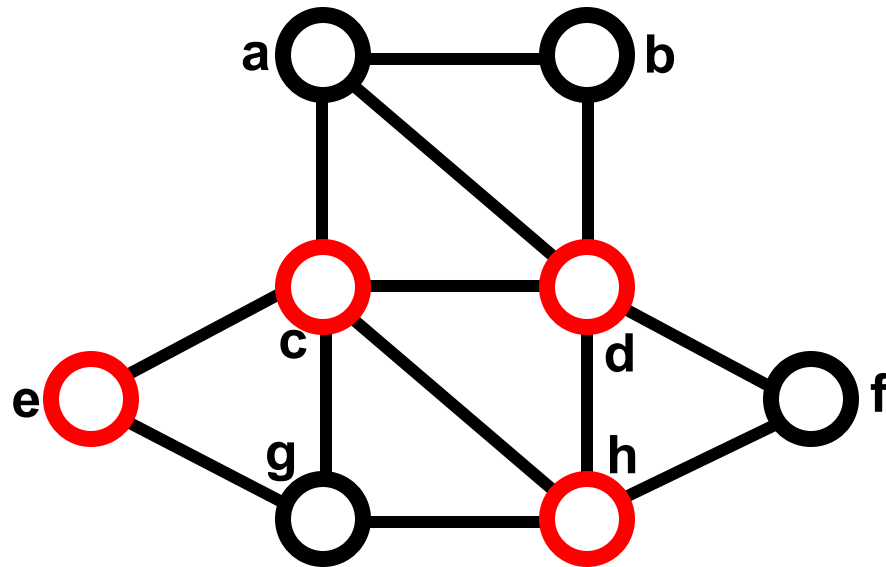
Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5); b, e (7); a

Simplified Fiduccia-Mattheyses: Example (9)

The unmoved node in Part2 with the largest gain (the only one) is h. We tentatively move it to Part1.

The cut size after the final tentative swap is 8, the same as it was before any tentative moves.



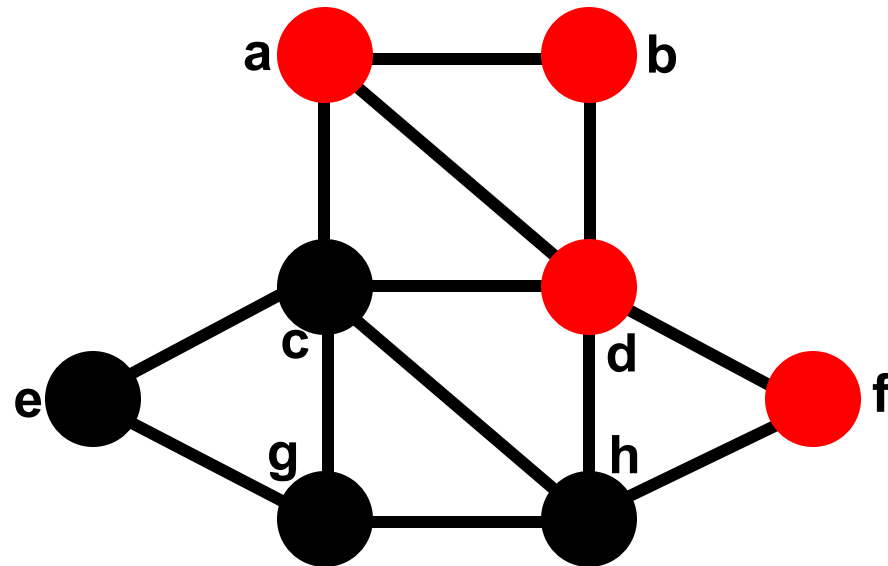
Nodes tentatively moved (and cut size after each pair):

none (8); g, d (4); f, c (5); b, e (7); a, h (8)

Simplified Fiduccia-Mattheyses: Example (10)

After every node has been tentatively moved, we look back at the sequence and see that the smallest cut was 4, after swapping g and d. We make that swap permanent and undo all the later tentative swaps.

This is the end of the first improvement step.



Nodes tentatively moved (and cut size after each pair):

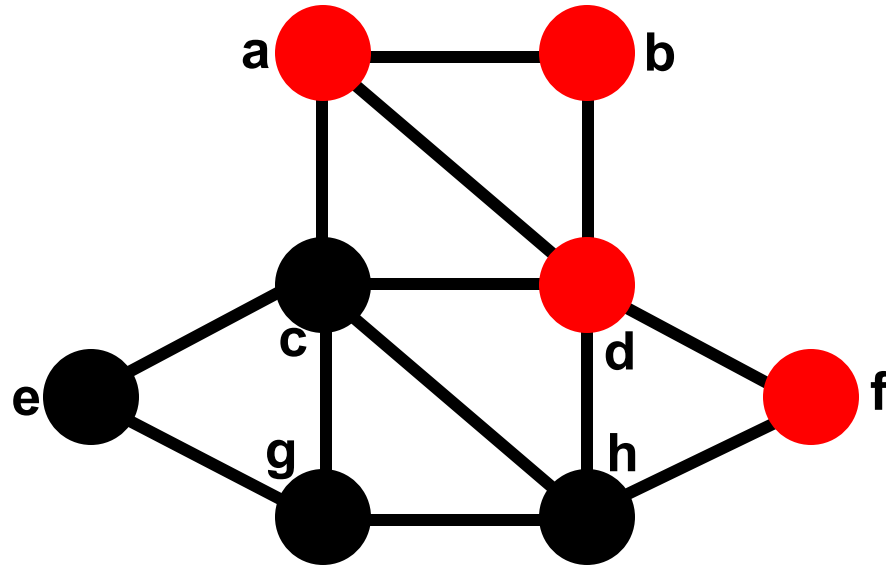
none (8); **g, d** (4); f, c (5); b, e (7); a, h (8)

Simplified Fiduccia-Mattheyses: Example (11)

Now we recompute the gains and do another improvement step starting from the new size-4 cut. The details are not shown.

The second improvement step doesn't change the cut size, so the algorithm ends with a cut of size 4.

In general, we keep doing improvement steps as long as the cut size keeps getting smaller.



Comments on Kernighan/Lin Algorithm

- Most expensive line shown in red, $O(n^3)$
- Some gain(k) may be negative, but if later gains are large, then final Gain may be positive
 - can escape “local minima” where switching no pair helps
- How many times do we Repeat?
 - K/L tested on very small graphs ($|N| \leq 360$) and got convergence after 2-4 sweeps
 - For random graphs (of theoretical interest) the probability of convergence in one step appears to drop like $2^{-|N|/30}$

A summary of improvements over Kernighan/Lin can be found in this recent survey:

Buluç, A., Meyerhenke, H., Safro, I., Sanders, P., & Schulz, C. (2016). Recent advances in graph partitioning. In Algorithm Engineering.

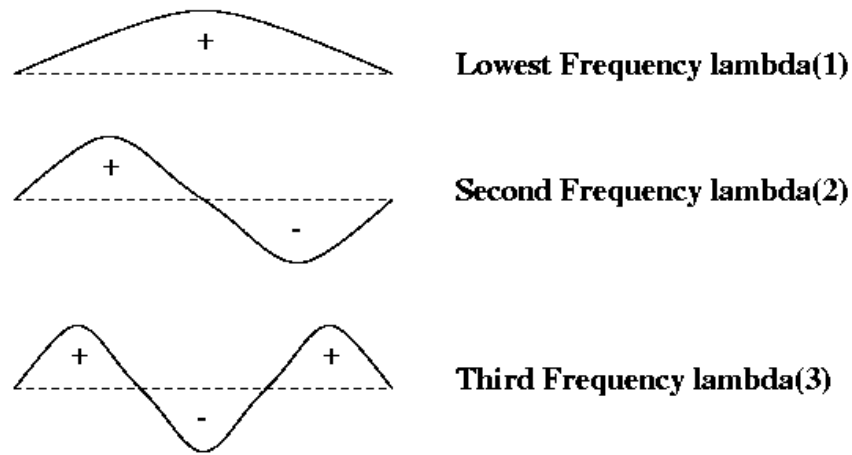
Coordinate-Free: Spectral Bisection

- Based on theory of Fiedler (1970s), popularized by Pothen, Simon, Liou (1990)
- Motivation, by analogy to a vibrating string
- Basic definitions
- Vibrating string, revisited
- Implementation via the Lanczos Algorithm
 - To optimize sparse-matrix-vector multiply, we graph partition
 - To graph partition, we find an eigenvector of a matrix associated with the graph
 - To find an eigenvector, we do sparse-matrix vector multiply
 - No free lunch ...

Motivation for Spectral Bisection

- Vibrating string
- Think of $G = 1D$ mesh as masses (nodes) connected by springs (edges), i.e. a string that can vibrate
- Vibrating string has **modes of vibration**, or **harmonics**
- Label nodes by whether mode - or + to partition into N_- and N_+
- Same idea for other graphs (eg planar graph \sim trampoline)

Modes of a Vibrating String



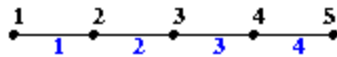
Basic Definitions

- *Definition:* The **incidence matrix $In(G)$** of a graph $G(N,E)$ is an $|N|$ by $|E|$ matrix, with one row for each node and one column for each edge. If edge $e=(i,j)$ then column e of $In(G)$ is zero except for the i -th and j -th entries, which are $+1$ and -1 , respectively.
- Slightly ambiguous definition because multiplying column e of $In(G)$ by -1 still satisfies the definition, but this won't matter...
- *Definition:* The **Laplacian matrix $L(G)$** of a graph $G(N,E)$ is an $|N|$ by $|N|$ symmetric matrix, with one row and column for each node. It is defined by
 - $L(G) (i,i) = \text{degree of node } i \text{ (number of incident edges)}$
 - $L(G) (i,j) = -1$ if $i \neq j$ and there is an edge (i,j)
 - $L(G) (i,j) = 0$ otherwise

Example of $\text{In}(G)$ and $\text{L}(G)$ for Simple Meshes

Incidence and Laplacian Matrices

Graph G

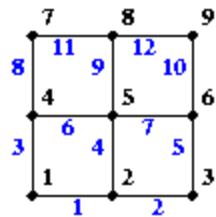


Incidence Matrix $\text{In}(G)$

$$\begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} -1 & & & \\ 1 & -1 & & \\ & 1 & -1 & \\ & & 1 & -1 \\ & & & 1 \end{bmatrix} \end{matrix}$$

Laplacian Matrix $\text{L}(G)$

$$\begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{bmatrix} 1 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & -1 & \\ & & -1 & 2 & -1 \\ & & & -1 & 1 \end{bmatrix} \end{matrix}$$



$$\begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{matrix} & \begin{bmatrix} -1 & & & 1 & & & & & & & & \\ 1 & -1 & & & 1 & & & & & & & \\ & 1 & -1 & & & 1 & & & & & & \\ & & 1 & -1 & & & -1 & 1 & & & & \\ & & & -1 & 1 & -1 & & 1 & & & & \\ & & & & -1 & 1 & -1 & & 1 & & & \\ & & & & & -1 & 1 & & & -1 & 1 & \\ & & & & & & -1 & 1 & -1 & & & \\ & & & & & & & -1 & 1 & & & \end{bmatrix} \end{matrix}$$

$$\begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \end{matrix} & \begin{bmatrix} 2 & -1 & -1 & & & & & & \\ -1 & 3 & -1 & -1 & & & & & \\ & -1 & 2 & & -1 & & & & \\ -1 & & & 3 & -1 & -1 & & & \\ & -1 & & -1 & 4 & -1 & -1 & & \\ & & -1 & -1 & 3 & & & -1 & \\ & & & -1 & & 2 & -1 & & \\ & & & & -1 & -1 & 3 & -1 & \\ & & & & & -1 & -1 & 2 \end{bmatrix} \end{matrix}$$

Nodes numbered in black

Edges numbered in blue

Properties of Laplacian Matrix

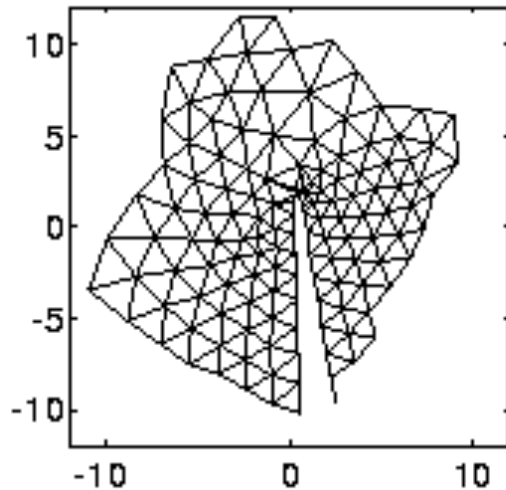
- *Theorem 1:* Given G , $L(G)$ has the following properties
(proof on 1996 CS267 web page)
 - $L(G)$ is symmetric.
 - This means the eigenvalues of $L(G)$ are real and its eigenvectors are real and orthogonal.
 - $\ln(G) * (\ln(G))^T = L(G)$
 - The eigenvalues of $L(G)$ are nonnegative:
 - $0 = \lambda_1 \leq \lambda_2 \leq \dots \leq \lambda_n$
 - The number of connected components of G is equal to the number of λ_i equal to 0.
 - *Definition:* $\lambda_2(L(G))$ is the algebraic connectivity of G
 - The magnitude of λ_2 measures connectivity
 - In particular, $\lambda_2 \neq 0$ if and only if G is connected.

Spectral Bisection Algorithm

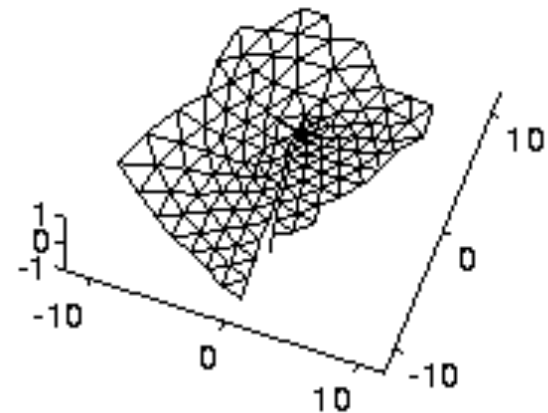
- Spectral Bisection Algorithm:
 - Compute eigenvector v_2 corresponding to $\lambda_2(L(G))$
 - For each node n of G
 - if $v_2(n) < 0$ put node n in partition N_-
 - else put node n in partition N_+
- Why does this make sense? Some reasons...
 - *Theorem 2 (Fiedler, 1975):* Let G be connected, and N_- and N_+ defined as above. Then N_- is connected. If no $v_2(n) = 0$, then N_+ is also connected. (proof on 1996 CS267 web page)
 - Recall $\lambda_2(L(G))$ is the algebraic connectivity of G
 - *Theorem 3 (Fiedler):* Let $G_1(N, E_1)$ be a subgraph of $G(N, E)$, so that G_1 is “less connected” than G . Then $\lambda_2(L(G_1)) \leq \lambda_2(L(G))$, i.e. the algebraic connectivity of G_1 is less than or equal to the algebraic connectivity of G . (proof on 1996 CS267 web page)

2nd eigenvector of L (planar mesh)

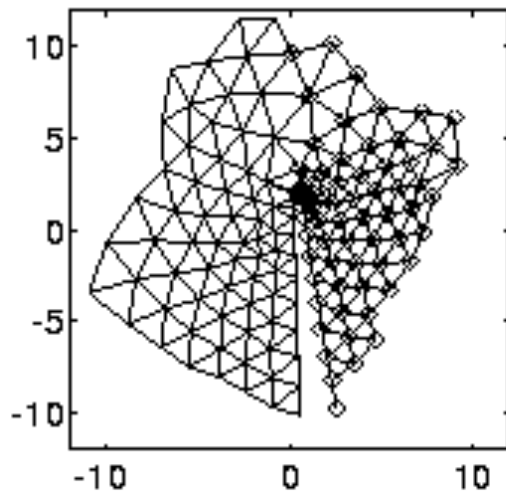
Original FE mesh



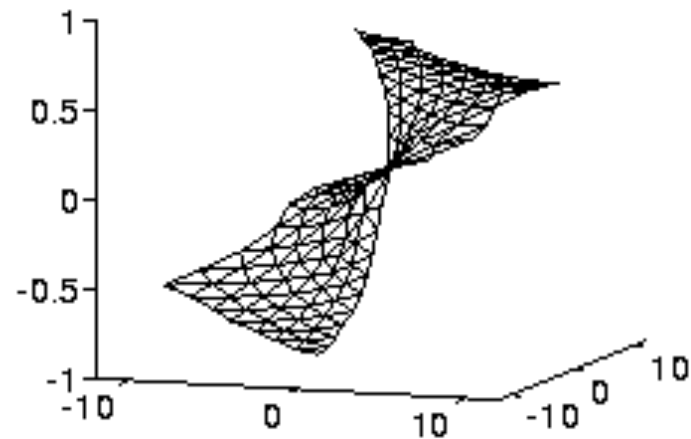
Plot of v_2 from above



Circle node i if $v_2(i) > 0$



Plot of v_2 head on



Computing v_2 and λ_2 of $L(G)$ using Lanczos

- Given any n -by- n symmetric matrix A (such as $L(G)$) Lanczos computes a k -by- k “approximation” T by doing k matrix-vector products, $k \ll n$

Choose an arbitrary starting vector r

$b(0) = \|r\|$

$j=0$

repeat

$j=j+1$

$q(j) = r/b(j-1)$

... scale a vector (BLAS1)

$r = A*q(j)$

... matrix vector multiplication, the most expensive step

$r = r - b(j-1)*v(j-1)$

... “axpy”, or scalar*vector + vector (BLAS1)

$a(j) = v(j)^T * r$

... dot product (BLAS1)

$r = r - a(j)*v(j)$

... “axpy” (BLAS1)

$b(j) = \|r\|$

... compute vector norm (BLAS1)

until convergence

... details omitted

$$T = \begin{pmatrix} a(1) & b(1) & & & & \\ b(1) & a(2) & b(2) & & & \\ & b(2) & a(3) & b(3) & & \\ & & \dots & \dots & \dots & \\ \bigcirc & & & b(k-2) & a(k-1) & b(k-1) \\ & & & & b(k-1) & a(k) \end{pmatrix}$$

- Approximate A 's eigenvalues/vectors using T 's

Spectral Bisection: Summary

- Laplacian matrix represents graph connectivity
- Second eigenvector gives a graph bisection
 - Roughly equal “weights” in two parts
 - Weak connection in the graph will be separator
- Implementation via the Lanczos Algorithm
 - To optimize sparse-matrix-vector multiply, we graph partition
 - To graph partition, we find an eigenvector of a matrix associated with the graph
 - To find an eigenvector, we do sparse-matrix vector multiply
- Have we made progress?
 - The first matrix-vector multiplies are slow, but use them to learn how to make the rest faster

Outline of Graph Partitioning Lectures

- Review definition of Graph Partitioning problem
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- Partitioning with Nodal Coordinates
 - Ex: In finite element models, node at point in (x,y) or (x,y,z) space
- Partitioning without Nodal Coordinates
 - Ex: In model of WWW, nodes are web pages
- **Multilevel Acceleration**
 - **BIG IDEA**, appears often in scientific computing
- Available Implementations
- Beyond Graph Partitioning: Hypergraphs

Introduction to Multilevel Partitioning

- If we want to partition $G(N,E)$, but it is too big to do efficiently, what can we do?
 - 1) Replace $G(N,E)$ by a coarse approximation $G_C(N_C,E_C)$, and partition G_C instead
 - 2) Use partition of G_C to get a rough partitioning of G , and then iteratively improve it
- What if G_C still too big?
 - Apply same idea recursively

Multilevel Partitioning - High Level Algorithm

$(N^+, N^-) = \text{Multilevel_Partition}(N, E)$

... recursive partitioning routine returns N^+ and N^- where $N = N^+ \cup N^-$

if $|N|$ is small

(1) Partition $G = (N, E)$ directly to get $N = N^+ \cup N^-$
Return (N^+, N^-)

else

(2) Coarsen G to get an approximation $G_c = (N_c, E_c)$

(3) $(N_c^+, N_c^-) = \text{Multilevel_Partition}(N_c, E_c)$

(4) Expand (N_c^+, N_c^-) to a partition (N^+, N^-) of N

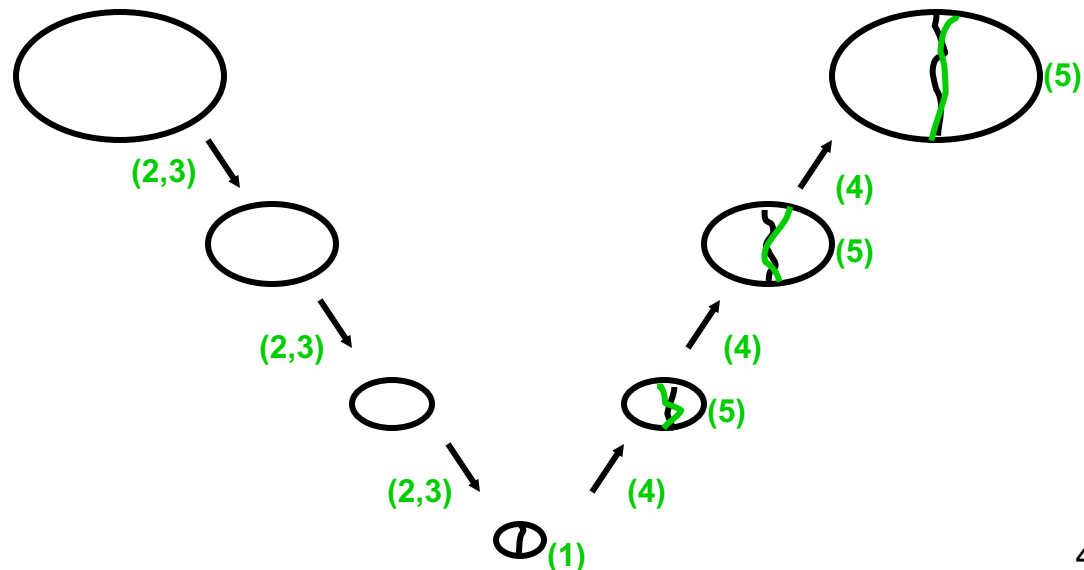
(5) Improve the partition (N^+, N^-)

Return (N^+, N^-)

endif

“V - cycle:”

How do we
Coarsen?
Expand?
Improve?



Multilevel Kernighan-Lin

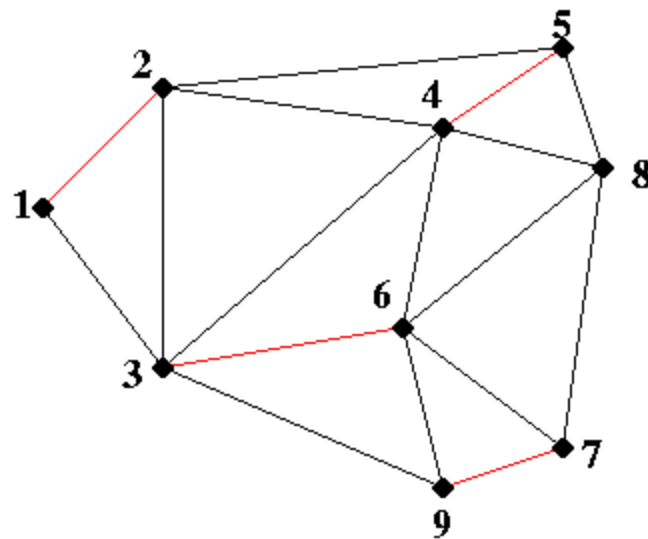
- Coarsen graph and expand partition using maximal matchings
- Improve partition using Kernighan-Lin

Maximal Matching

- *Definition:* A **matching** of a graph $G(N,E)$ is a subset E_m of E such that no two edges in E_m share an endpoint
- *Definition:* A **maximal matching** of a graph $G(N,E)$ is a matching E_m to which no more edges can be added and remain a matching
- A simple greedy algorithm computes a maximal matching:

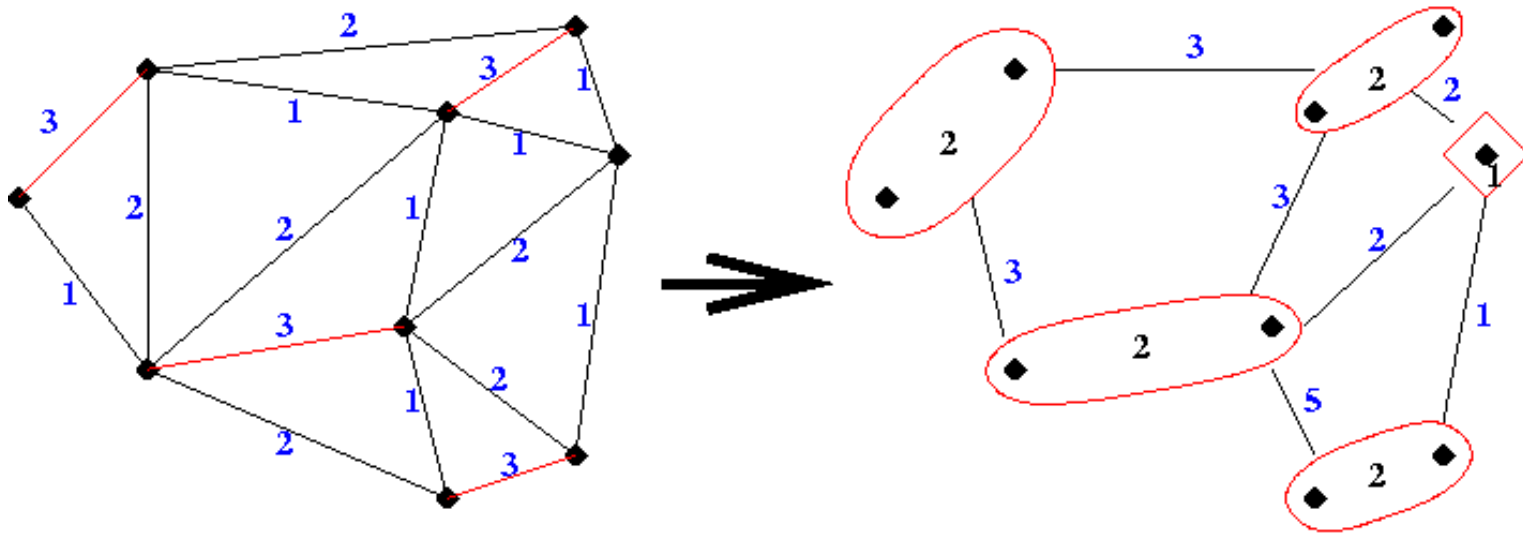
```
let  $E_m$  be empty
mark all nodes in  $N$  as unmatched
for  $i = 1$  to  $|N|$     ... visit the nodes in any order
    if  $i$  has not been matched
        mark  $i$  as matched
        if there is an edge  $e=(i,j)$  where  $j$  is also unmatched,
            add  $e$  to  $E_m$ 
            mark  $j$  as matched
        endif
    endif
endfor
```

Maximal Matching: Example



Example of Coarsening

How to coarsen a graph using a maximal matching



$G = (N, E)$

E_m is shown in red

Edge weights shown in blue

Node weights are all one

$G_c = (N_c, E_c)$

N_c is shown in red

Edge weights shown in blue

Node weights shown in black

Coarsening using a maximal matching (details)

1) Construct a maximal matching E_m of $G(N,E)$

for all edges $e=(j,k)$ in E_m

2) collapse matched nodes into a single one

Put node $n(e)$ in N_c

$W(n(e)) = W(j) + W(k)$... gray statements update node/edge weights

for all nodes n in N not incident on an edge in E_m 3) add unmatched nodes

Put n in N_c ... do not change $W(n)$

... Now each node r in N is “inside” a unique node $n(r)$ in N_c

... 4) Connect two nodes in N_c if nodes inside them are connected in E

for all edges $e=(j,k)$ in E_m

for each other edge $e'=(j,r)$ or (k,r) in E

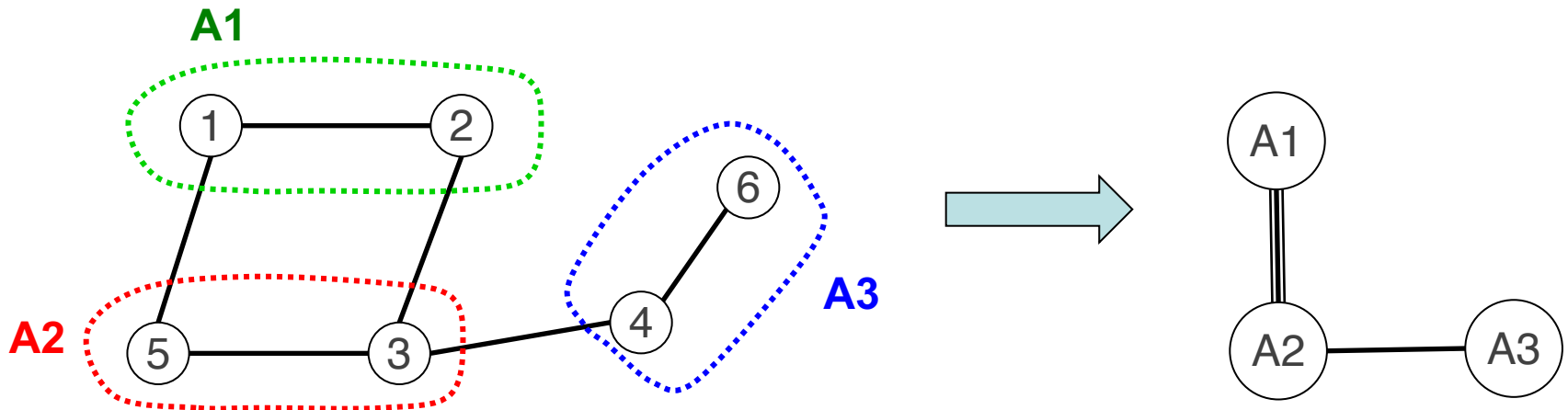
Put edge $ee = (n(e),n(r))$ in E_c

$W(ee) = W(e')$

If there are multiple edges connecting two nodes in N_c , collapse them,
adding edge weights

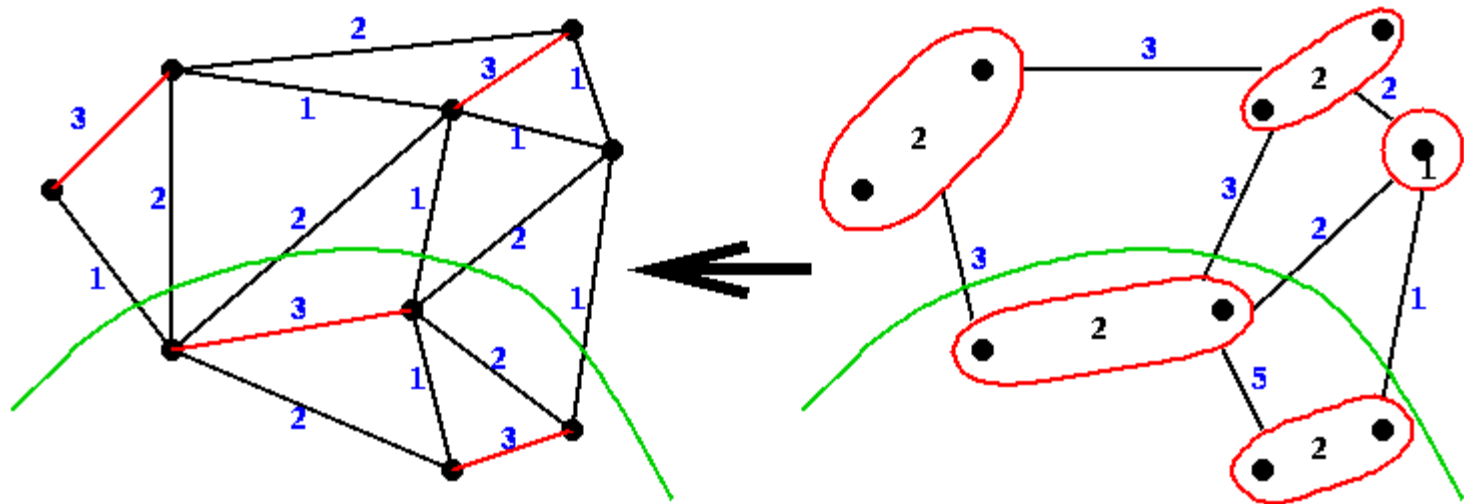
Coarsening via sparse matrix-matrix products

$$\begin{bmatrix} 1 & 1 & & & & \\ & & 1 & & 1 & \\ & & & 1 & & \\ & & & & 1 & 1 \end{bmatrix} \times \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{matrix} & \begin{bmatrix} & \bullet & & & \bullet & \\ \bullet & & \bullet & & & \\ & \bullet & & \bullet & \bullet & \\ & & \bullet & & & \bullet \\ \bullet & & \bullet & & & \\ & & & \bullet & & \end{bmatrix} \end{matrix} \times \begin{bmatrix} 1 & & & & & \\ 1 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 \end{bmatrix} = \begin{bmatrix} & 2 & & & & \\ 2 & & & & & \\ & 1 & & & & \\ & & 1 & & & \\ & & & 1 & & \\ & & & & 1 \end{bmatrix}$$



Expanding a partition of G_c to a partition of G

Converting a coarse partition to a fine partition



Partition shown in green

Multilevel Spectral Bisection

- Coarsen graph and expand partition using maximal independent sets
- Improve partition using Rayleigh Quotient Iteration

Maximal Independent Sets

- *Definition:* An **independent set** of a graph $G(N,E)$ is a subset N_i of N such that no two nodes in N_i are connected by an edge
- *Definition:* A **maximal independent set (MIS)** of a graph $G(N,E)$ is an independent set N_i to which no more nodes can be added and remain an independent set
- A simple greedy algorithm computes a maximal independent set:

```
let  $N_i$  be empty
for  $k = 1$  to  $|N|$     ... visit the nodes in any order
    if node  $k$  is not adjacent to any node already in  $N_i$ 
        add  $k$  to  $N_i$ 
    endif
endfor
```



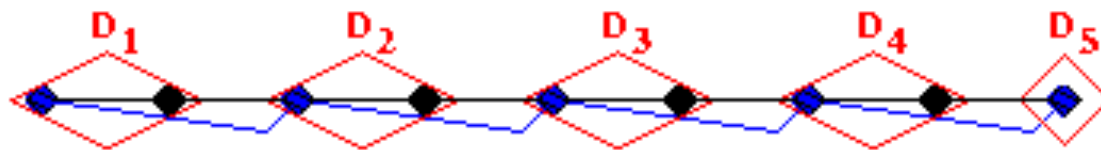
◆ and ◆ - nodes of N

◆ - nodes of N_i

- We will see parallel MIS in the graph algorithms class next week

Example of Coarsening

Computing G_c from G



◆ and ◆ - nodes of N

◆ - nodes of N_i

— - edges in E

— - edges in E_c

◆ - encloses domain $D_k = \text{node of } N_c$

Coarsening using Maximal Independent Sets (details)

... Build “domains” $D(k)$ around each node k in N_i to get nodes in N_c

... Add an edge to E_c whenever it would connect two such domains

E_c = empty set

for all nodes k in N_i

$D(k) = (\{k\}, \text{empty set})$

... first set contains nodes in $D(k)$, second set contains edges in $D(k)$

unmark all edges in E

repeat

choose an unmarked edge $e = (k,j)$ from E

if exactly one of k and j (say k) is in some $D(m)$

mark e

add j and e to $D(m)$

else if k and j are in two different $D(m)$'s (say $D(m_k)$ and $D(m_j)$)

mark e

add edge (m_k, m_j) to E_c

else if both k and j are in the same $D(m)$

mark e

add e to $D(m)$

else

leave e unmarked

endif

until no unmarked edges

Expanding a partition of G_c to a partition of G

- Need to convert an eigenvector v_c of $L(G_c)$ to an approximate eigenvector v of $L(G)$
- Use interpolation:

For each node j in N

if j is also a node in N_c , then

$v(j) = v_c(j)$... use same eigenvector component

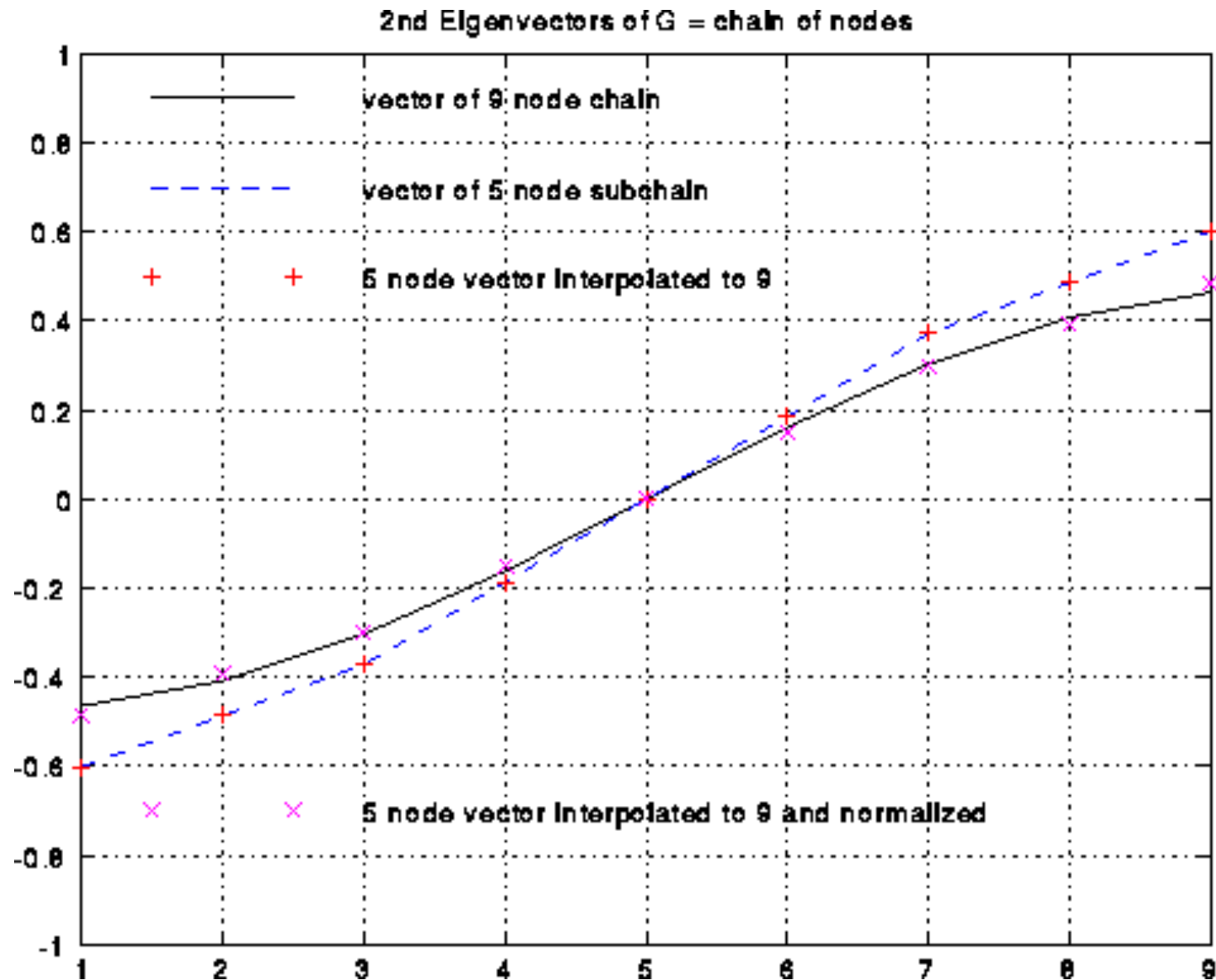
else

$v(j) = \text{average of } v_c(k) \text{ for all neighbors } k \text{ of } j \text{ in } N_c$

end if

endif

Example: 1D mesh of 9 nodes



Improve eigenvector: Rayleigh Quotient Iteration

$j = 0$

pick starting vector $v(0)$... from expanding v_c

repeat

$j=j+1$

$$r(j) = v^T(j-1) * L(G) * v(j-1)$$

... $r(j) = \text{Rayleigh Quotient of } v(j-1)$

... = good approximate eigenvalue

$$v(j) = (L(G) - r(j)*I)^{-1} * v(j-1)$$

... expensive to do exactly, so solve approximately

... using an iteration called SYMMLQ,

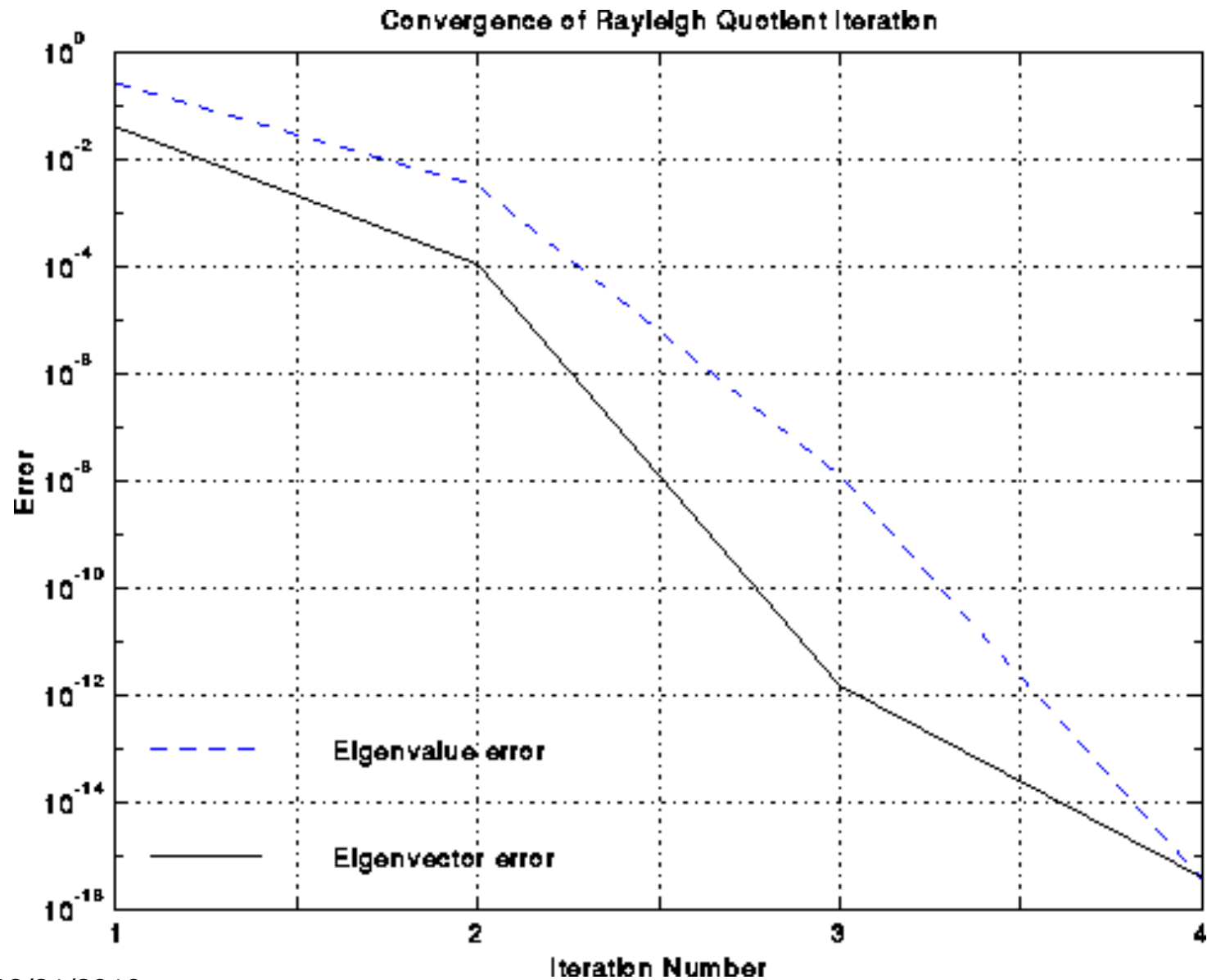
... which uses matrix-vector multiply (no surprise)

$$v(j) = v(j) / || v(j) || \quad \dots \text{normalize } v(j)$$

until $v(j)$ converges

... Convergence is very fast: cubic

Example of cubic convergence for 1D mesh



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- Review definition of Graph Partitioning problem
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 - Ex: In model of WWW, nodes are web pages
- Multilevel Acceleration
 - BIG IDEA, appears often in scientific computing
- **Available Implementations**
- Beyond Graph Partitioning: Hypergraphs

Available Implementations

- **Multilevel Kernighan/Lin**
 - METIS and ParMETIS (glaros.dtc.umn.edu/gkhome/views/metis)
 - SCOTCH and PT-SCOTCH (www.labri.fr/perso/pelegrin/scotch/)
- **Matlab toolbox for geometric and spectral partitioning by Gilbert, Tang, and Li:** <https://github.com/YingzhouLi/meshpart>
- **Multilevel Spectral Bisection**
 - S. Barnard and H. Simon, “A fast multilevel implementation of recursive spectral bisection ...”, 1993
 - Chaco (SC’14 Test of Time Award)
- **Hybrids possible**
 - Ex: Use Kernighan/Lin to improve a partition from spectral bisection
- **Recent packages with collection of techniques**
 - Zoltan (www.cs.sandia.gov/Zoltan)
 - KaHIP (<http://algo2.iti.kit.edu/kahip/>)

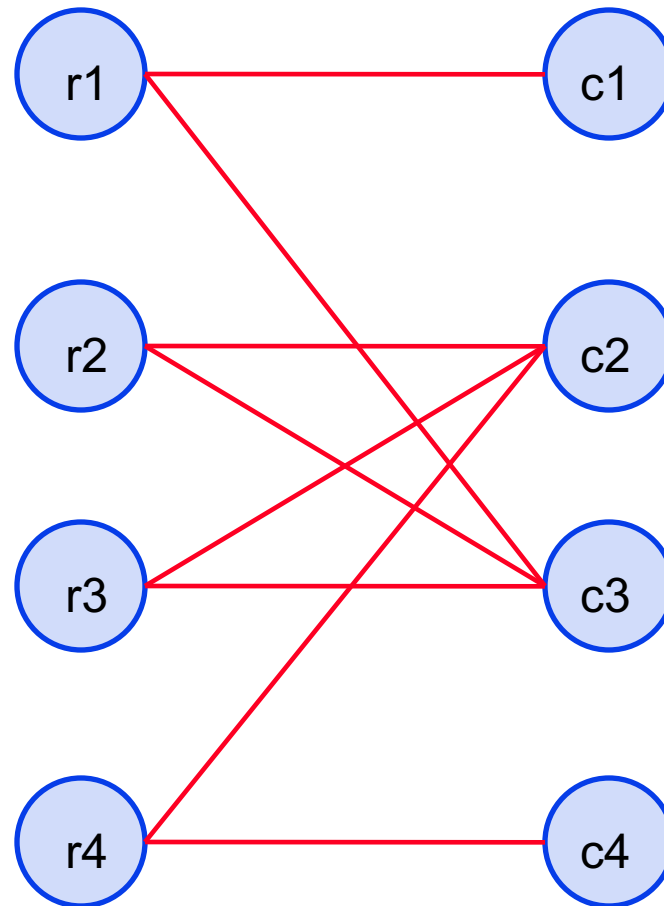
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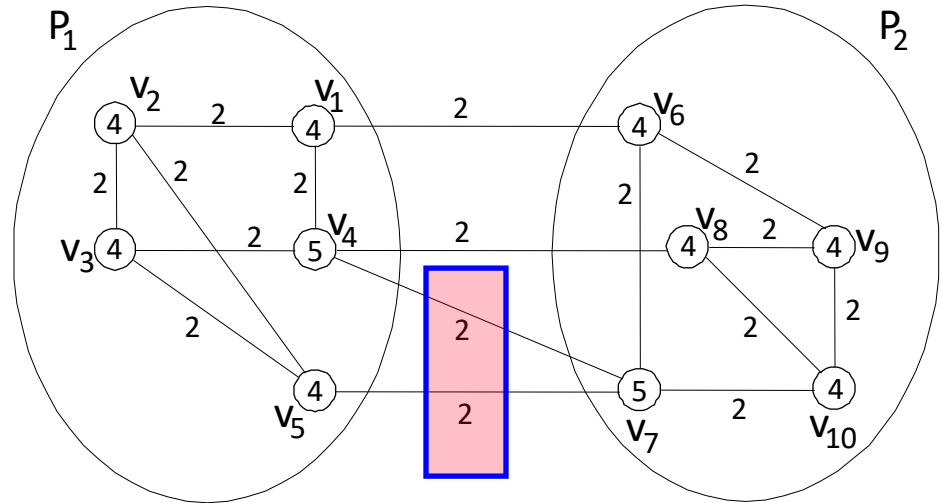
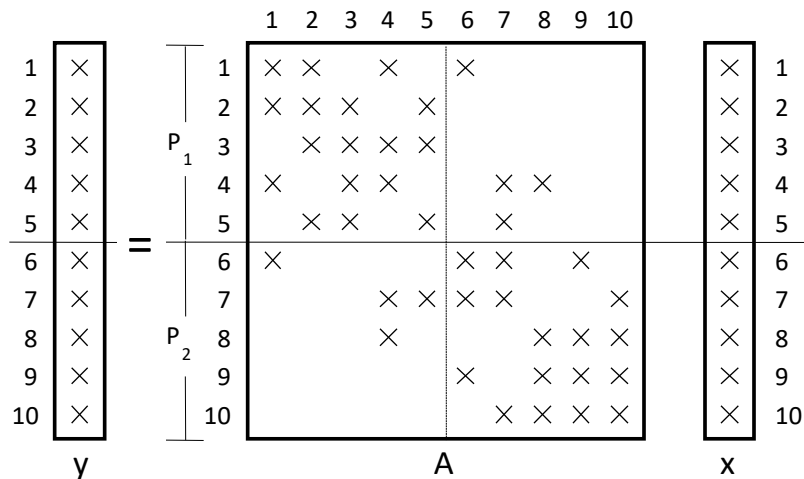
Beyond simple graph partitioning:

Representing a sparse matrix as a hypergraph

$$\begin{bmatrix} \times & 0 & \times & 0 \\ 0 & \times & \times & 0 \\ 0 & \times & \times & 0 \\ 0 & \times & 0 & \times \end{bmatrix}$$



A sparse matrix in the graph model



edge $(v_i, v_j) \in E \Rightarrow$

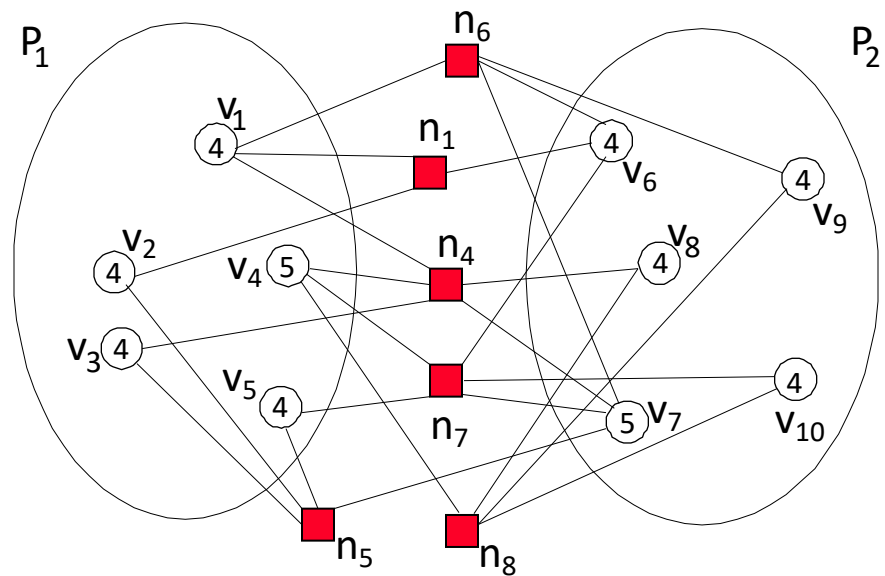
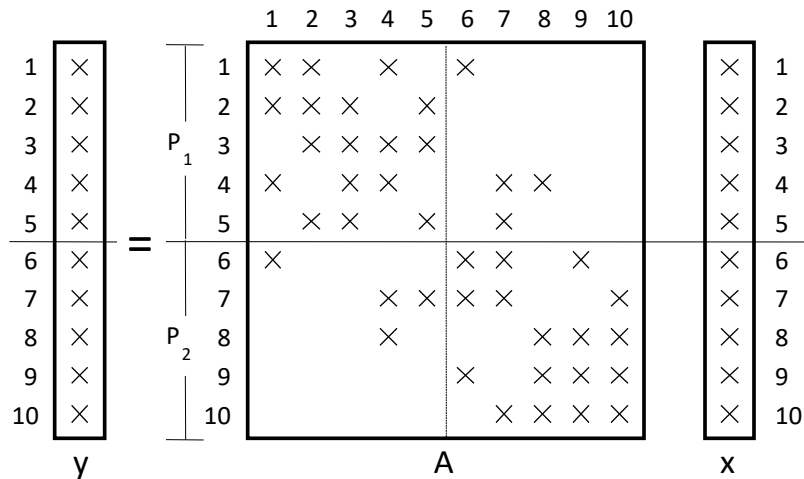
$$y(i) \leftarrow y(i) + A(i,j) x(j) \text{ and } y(j) \leftarrow y(j) + A(j,i) x(i)$$

P_1 performs: $y(4) \leftarrow y(4) + A(4,7) x(7)$ and

$$y(5) \leftarrow y(5) + A(5,7) x(7)$$

$x(7)$ only needs to be communicated **once** !

A sparse matrix in the hypergraph model



- Column-net model for block-row distributions
- Rows are vertices, columns are nets (hyperedges)

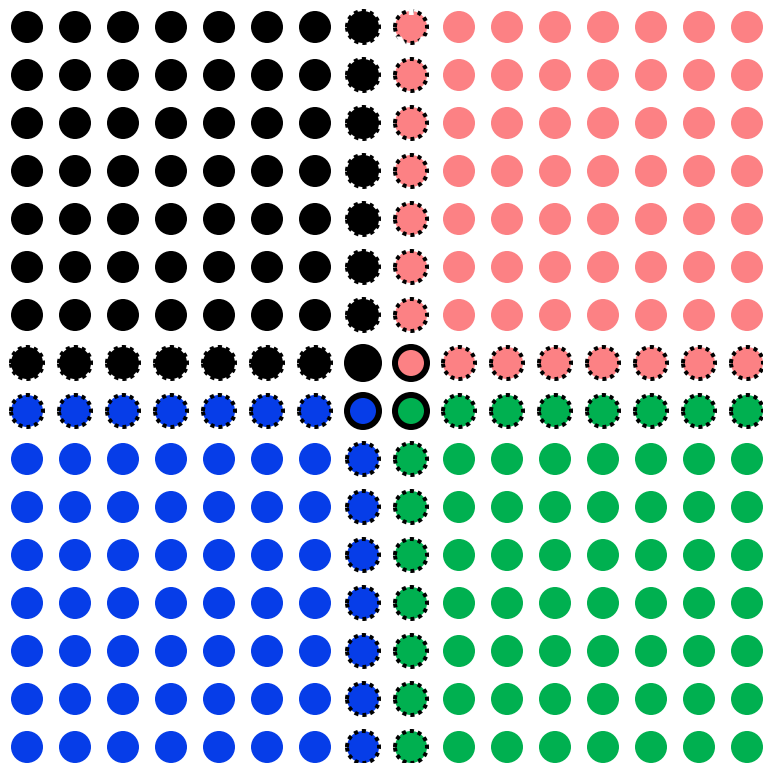
Each {vertex, net} pair represents unique nonzero net-cut metric:
 $\text{cutsizes}(\Pi) = \sum_{n \in NE} w(n_i)$

connectivity-1 metric: $\text{cutsizes}(\Pi) = \sum_{n \in NE} w(n_i) (c(n_i) - 1)$

Two Different 2D Mesh Partitioning Strategies

Graph:

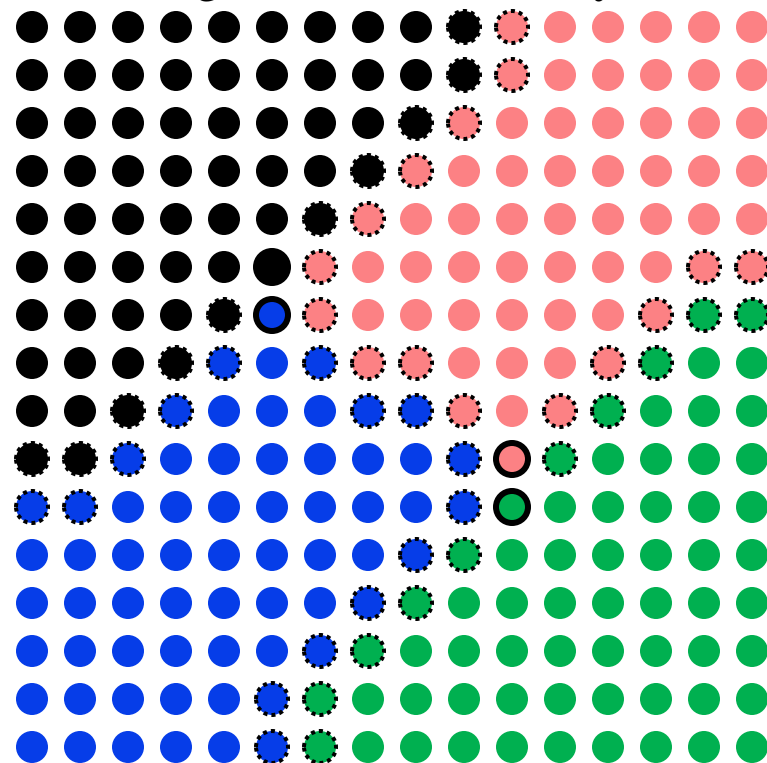
Cartesian Partitioning



Total SpMV communication volume = 64

Hypergraph:

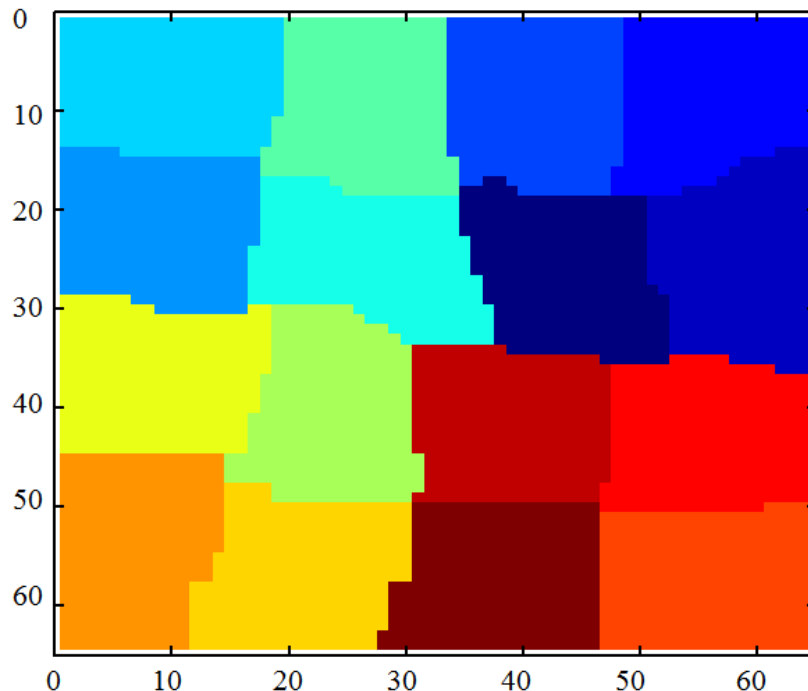
MeshPart Algorithm [Ucar, Catalyurek, 2010]



Total SpMV communication volume = 58

Experimental Results: Hypergraph vs. Graph Partitioning

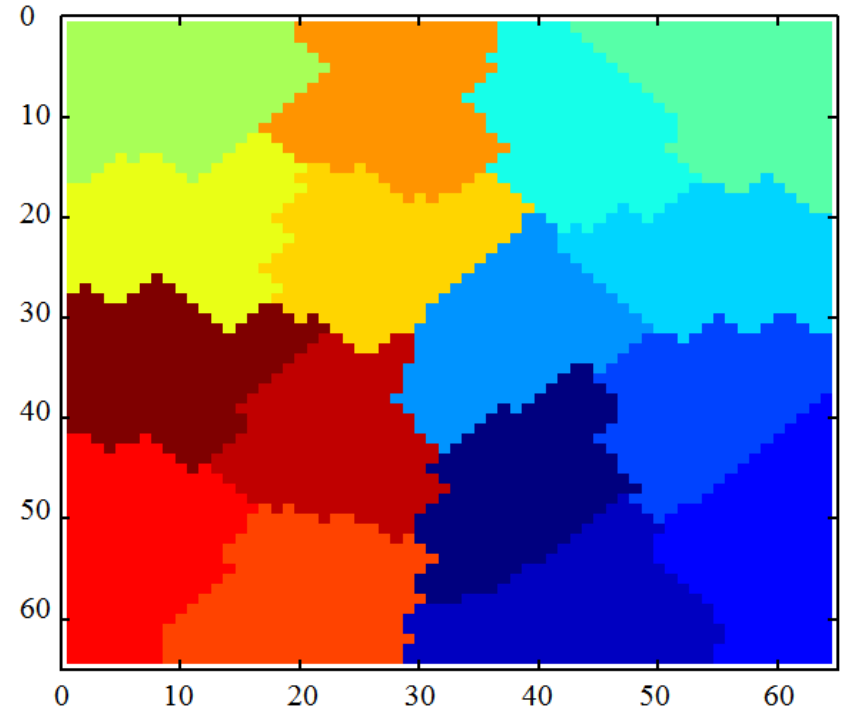
64x64 Mesh (5-pt stencil), 16 processors



Graph Partitioning (Metis)

Total Comm. Vol = 777

Max Vol per Proc = 69



Hypergraph Partitioning (PaToH)

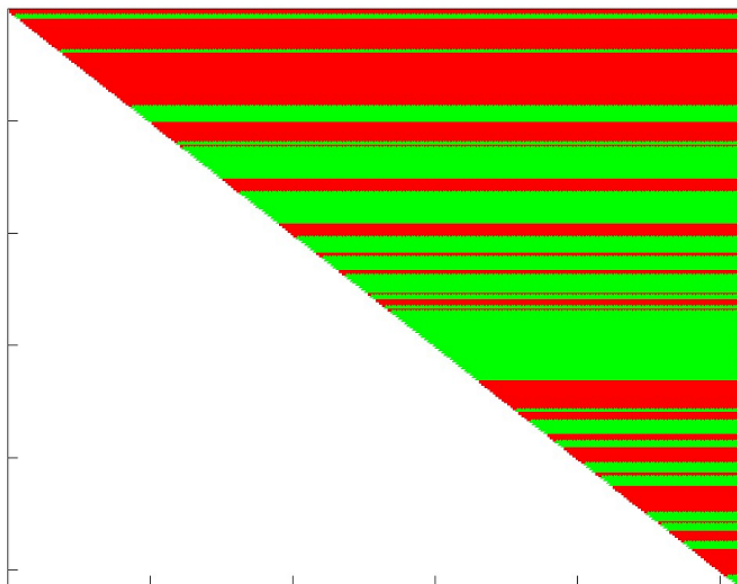
Total Comm. Vol = 719

Max Vol per Proc = 59

**~8% reduction in total communication volume
using hypergraph partitioning (PaToH)
versus graph partitioning (METIS)**

Further Benefits of Hypergraph Model: Nonsymmetric Matrices

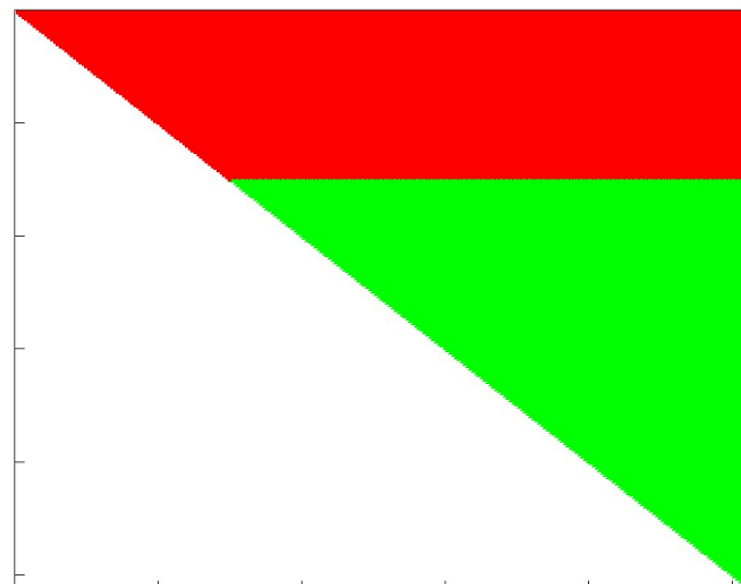
- Graph model of matrix has edge (i,j) if either $A(i,j)$ or $A(j,i)$ nonzero
- Same graph for A as $|A| + |A^T|$
- Ok for symmetric matrices, what about nonsymmetric?
 - Try A upper triangular



Graph Partitioning (Metis)

Total Communication Volume= 254

Load imbalance ratio = 6%



Hypergraph Partitioning (PaToH)

Total Communication Volume= 181

Load imbalance ratio = 0.1%

Summary: Graphs versus Hypergraphs

- Pros and cons
 - When matrix is non-symmetric, the graph partitioning model (using $A+A^T$) loses information, resulting in suboptimal partitioning in terms of communication and load balance.
 - Even when matrix is symmetric, graph cut size is not an accurate measurement of communication volume
 - Hypergraph partitioning model solves both these problems
 - However, hypergraph partitioning (PaToH) can be much more expensive than graph partitioning (METIS)
- Hypergraph partitioners: PaToH, HMETIS, ZOLTAN

Is Graph Partitioning a Solved Problem?

- Myths of partitioning due to Bruce Hendrickson
 - ➡ 1. Edge cut = communication cost
 - ➡ 2. Simple graphs are sufficient
 - ➡ 3. Edge cut is the right metric
 - 4. Existing tools solve the problem
 - 5. Key is finding the right partition
 - 6. Graph partitioning is a solved problem
- Slides and myths based on Bruce Hendrickson's:
“Load Balancing Myths, Fictions & Legends”

Myth: Partition Quality is Paramount

- When structure are changing dynamically during a simulation, need to partition dynamically
 - Speed may be more important than quality
 - **Partitioner must run fast in parallel**
 - Another chicken and egg problem here
 - Partition should be incremental
 - Change minimally relative to prior one
 - Must not use too much memory
- Recent research on streaming partitioning:
 - Stanton, I. and Kliot, G., “Streaming graph partitioning for large distributed graphs”. KDD, 2012.
 - The idea is used by many graph processing systems such as PowerGraph and GPS