
CS 267: Applications of Parallel Computers

Graph Partitioning

James Demmel

www.cs.berkeley.edu/~demmel/cs267_Spr12

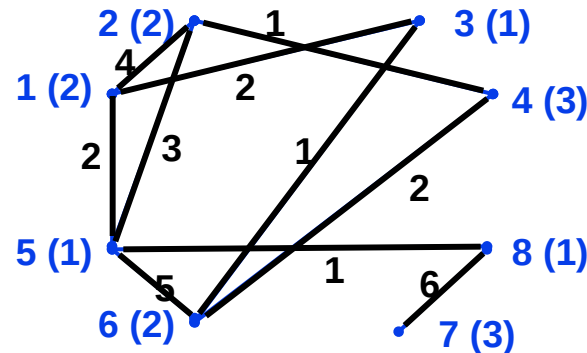
Outline of Graph Partitioning Lecture

- 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
- Comparison of Methods and Applications
- Beyond Graph Partitioning: Hypergraphs

Definition of Graph Partitioning

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

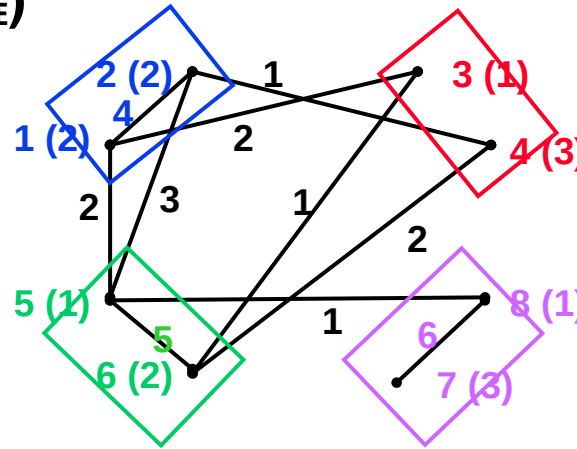
- N = nodes (or vertices),
- W_N = node weights
- E = edges
- W_E = edge weights



- 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

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**



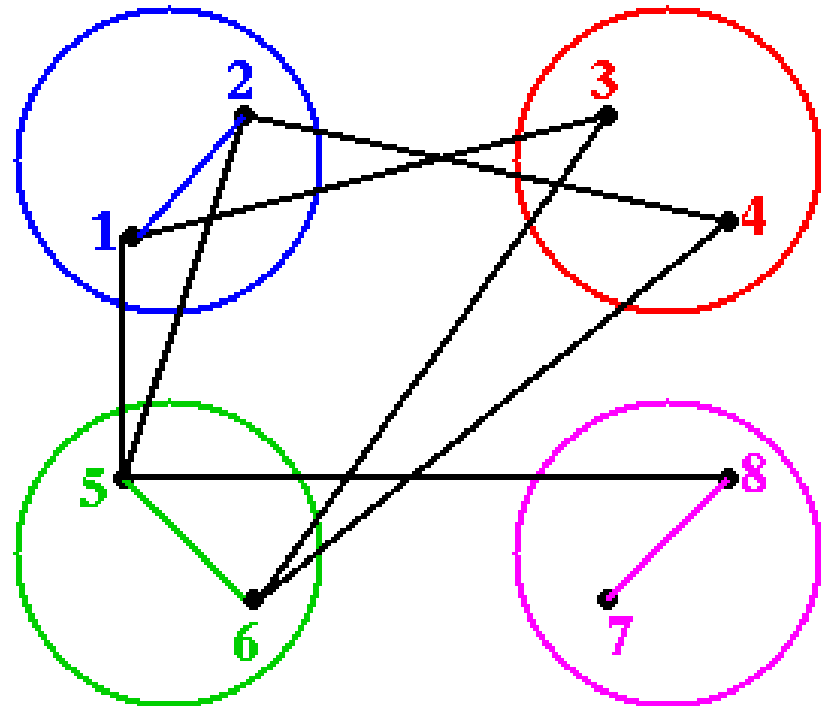
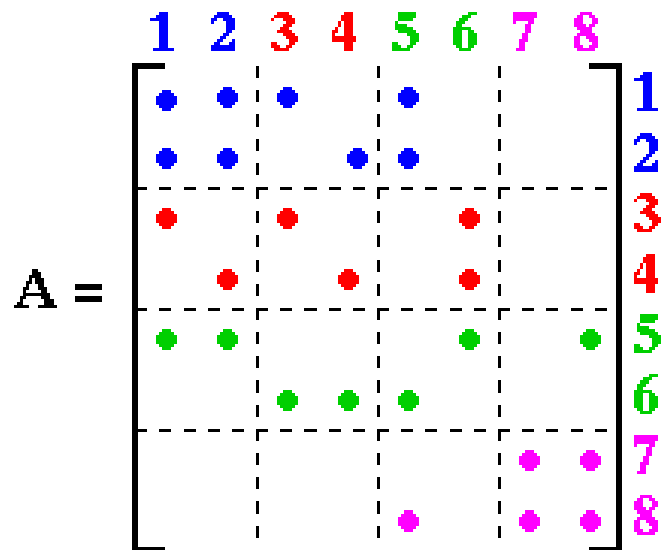
- **Ex: $N = \{\text{tasks}\}$, $W_N = \{\text{task costs}\}$, edge (j,k) in E means task j sends $W_E(j,k)$ words to task k**
- **Choose a partition $N = N_1 \cup N_2 \cup \dots \cup N_p$ such that**
 - **The sum of the node weights in each N_j is “about the same”**
 - **The sum of all edge weights of edges connecting all different pairs N_j and N_k is minimized (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 $y = y + A*x$

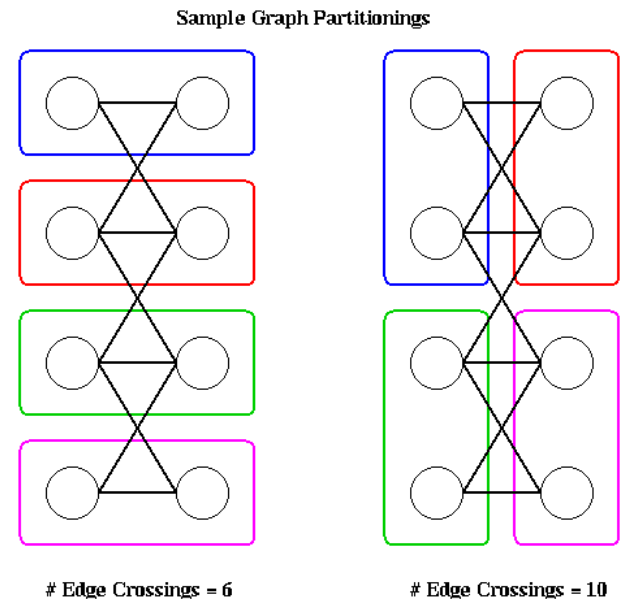
Partitioning a Sparse Symmetric Matrix



```
... 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

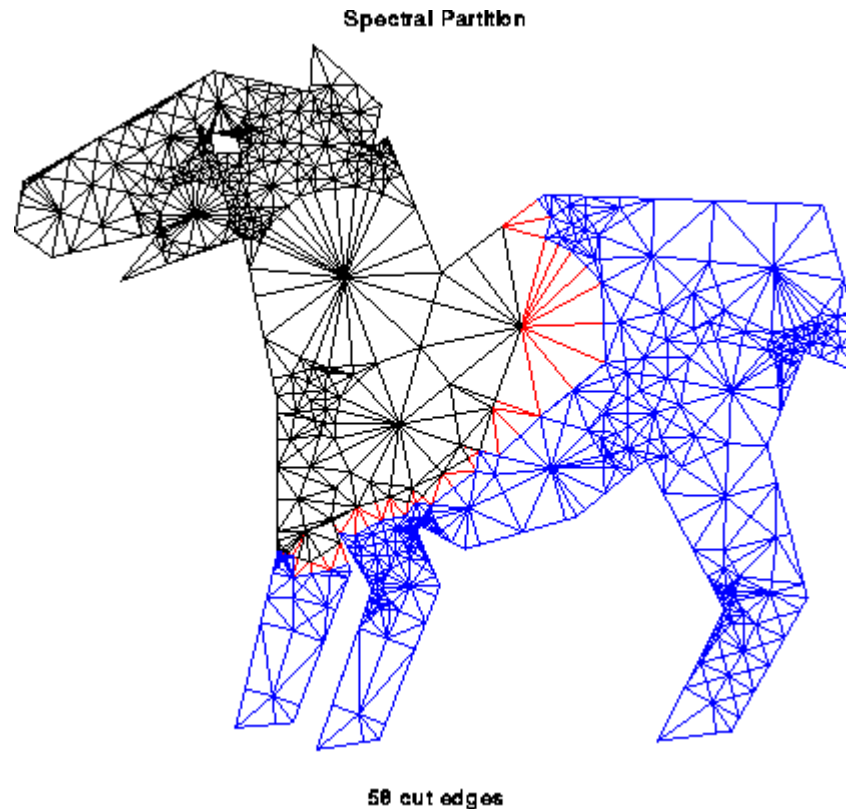
Outline of Graph Partitioning

Lectures

- 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
- Comparison of Methods and Applications
- Beyond Graph Partitioning: Hypergraphs

First Heuristic: Repeated Graph Bisection

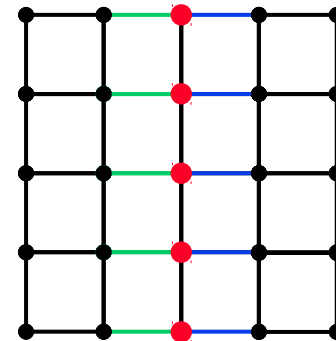
- To partition N into 2^k parts
 - bisect graph recursively k times
- Henceforth discuss mostly graph bisection



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

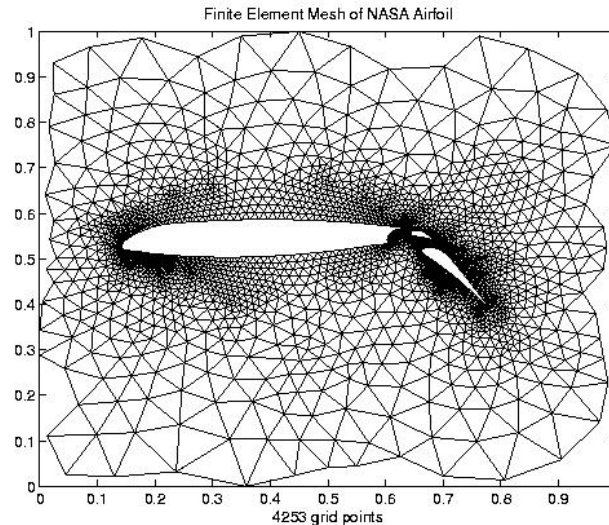
- $|N_s| \leq |E_s|$

- 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

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

Outline of Graph Partitioning

Lectures

- 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
- Comparison of Methods and Applications
- Beyond Graph Partitioning: Hypergraphs

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

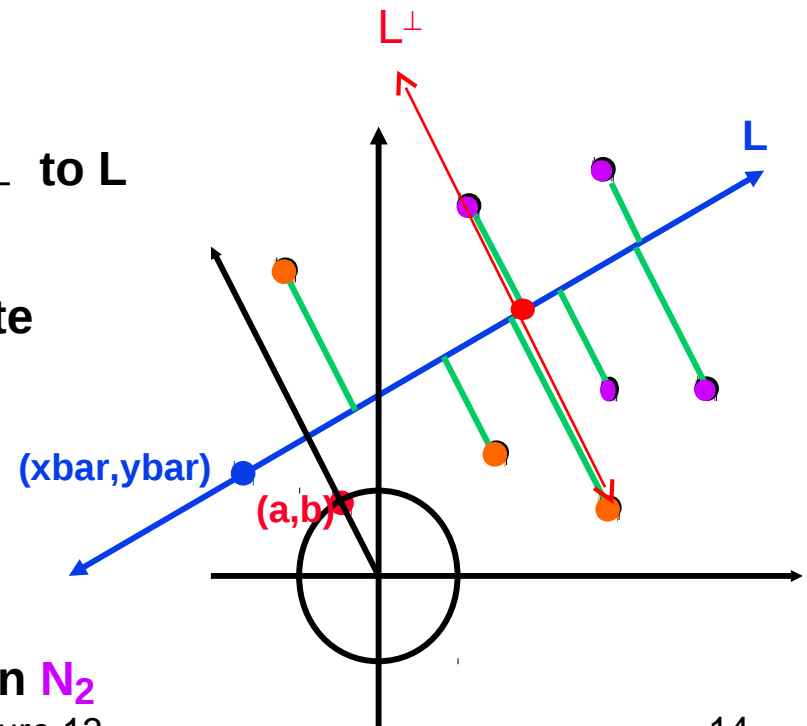
$$S_j = -b*(x_j - \bar{x}) + a*(y_j - \bar{y}) \text{ along } L$$

3. Compute the median

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

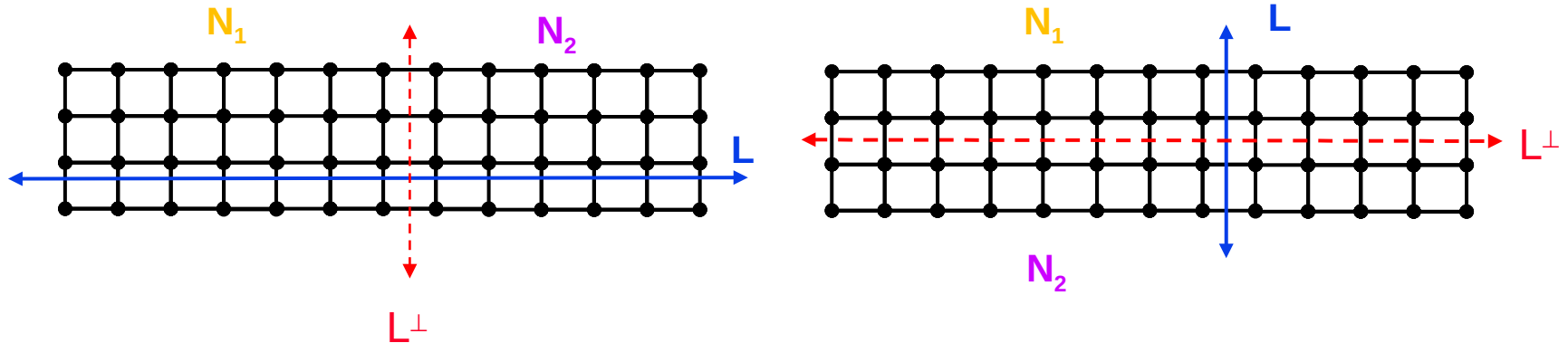
4. Use median to partition the nodes

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



Inertial Partitioning: Choosing L

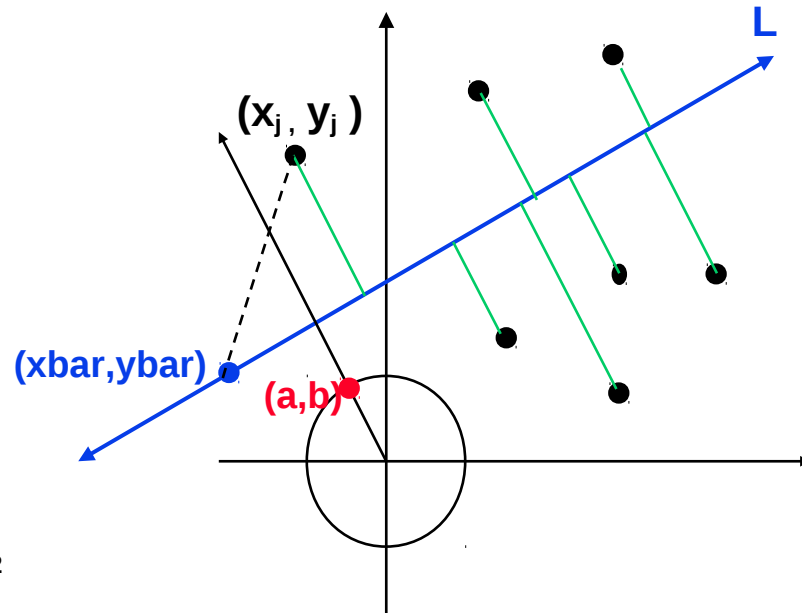
- Clearly prefer L, L^\perp on left below



- 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



Σ_j (length of j-th green line)²

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

... **Pythagorean Theorem**

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

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

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

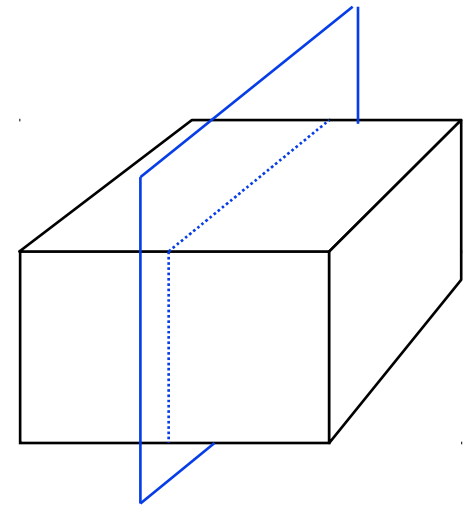
Minimized by choosing

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

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

Nodal Coordinates: Random Spheres

- Generalize nearest neighbor idea of a planar graph to higher dimensions
 - Any graph can fit in 3D without edge crossings
 - Capture intuition of planar graphs of being connected to “nearest neighbors” but in higher than 2 dimensions
- For intuition, consider graph defined by a regular 3D mesh
- An n by n by n mesh of $|N| = n^3$ nodes
 - Edges to 6 nearest neighbors
 - Partition by taking plane parallel to 2 axes
 - Cuts $n^2 = |N|^{2/3} = O(|E|^{2/3})$ edges
- For the general graphs
 - Need a notion of “well-shaped” like mesh

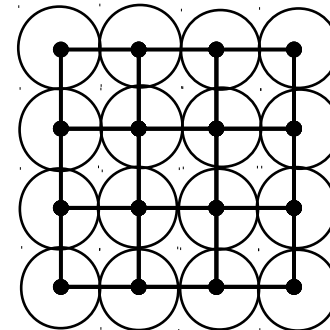


Random Spheres: Well Shaped Graphs

- Approach due to Miller, Teng, Thurston, Vavasis
- **Def:** A **k-ply neighborhood system in d dimensions** is a set $\{D_1, \dots, D_n\}$ of closed disks in R^d such that no point in R^d is strictly interior to more than k disks
- **Def:** An **(α, k) overlap graph** is a graph defined in terms of $\alpha \geq 1$ and a k-ply neighborhood system $\{D_1, \dots, D_n\}$: There is a node for each D_j , and an edge from j to i if expanding the radius of the smaller of D_j and D_i by $>\alpha$ causes the two disks to overlap

Ex: n-by-n mesh is a (1,1) overlap graph

Ex: Any planar graph is (α, k) overlap for some α, k



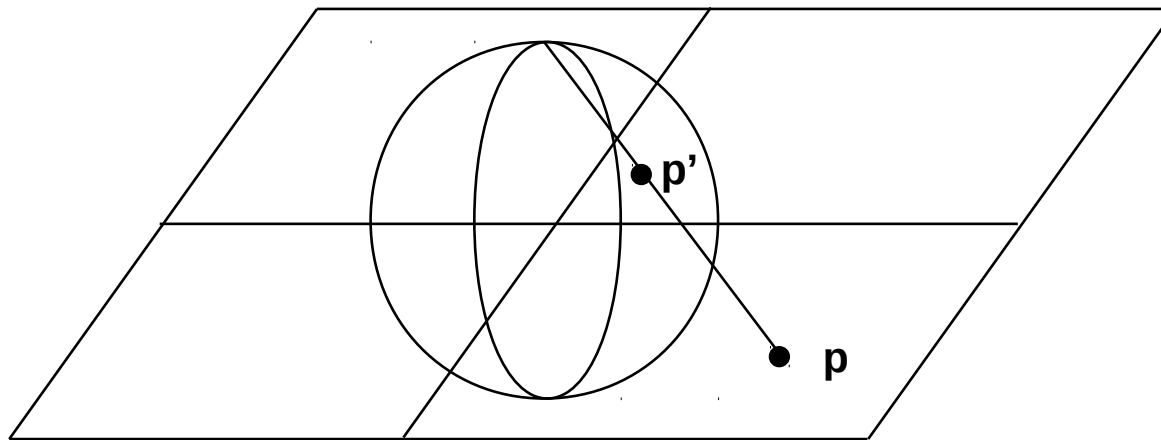
**2D Mesh is
(1,1) overlap
graph**

Generalizing Lipton/Tarjan to Higher Dimensions

- *Theorem* (Miller, Teng, Thurston, Vavasis, 1993):
Let $G=(N,E)$ be an (α,k) overlap graph in d dimensions with $n=|N|$. Then there is a vertex separator N_s such that
 - $N = N_1 \cup N_s \cup N_2$ and
 - N_1 and N_2 each has at most $n \cdot (d+1)/(d+2)$ nodes
 - N_s has at most $O(\alpha \cdot k^{1/d} \cdot n^{(d-1)/d})$ nodes
- When $d=2$, same as Lipton/Tarjan
- Algorithm:
 - Choose a sphere S in R^d
 - Edges that S “cuts” form edge separator E_s
 - Build N_s from E_s
 - Choose S “randomly”, so that it satisfies Theorem with high

Stereographic Projection

- Stereographic projection from plane to sphere
 - In $d=2$, draw line from p to North Pole, projection p' of p is where the line and sphere intersect



$$p = (x, y)$$

$$p' = (2x, 2y, x^2 + y^2 - 1) / (x^2 + y^2 + 1)$$

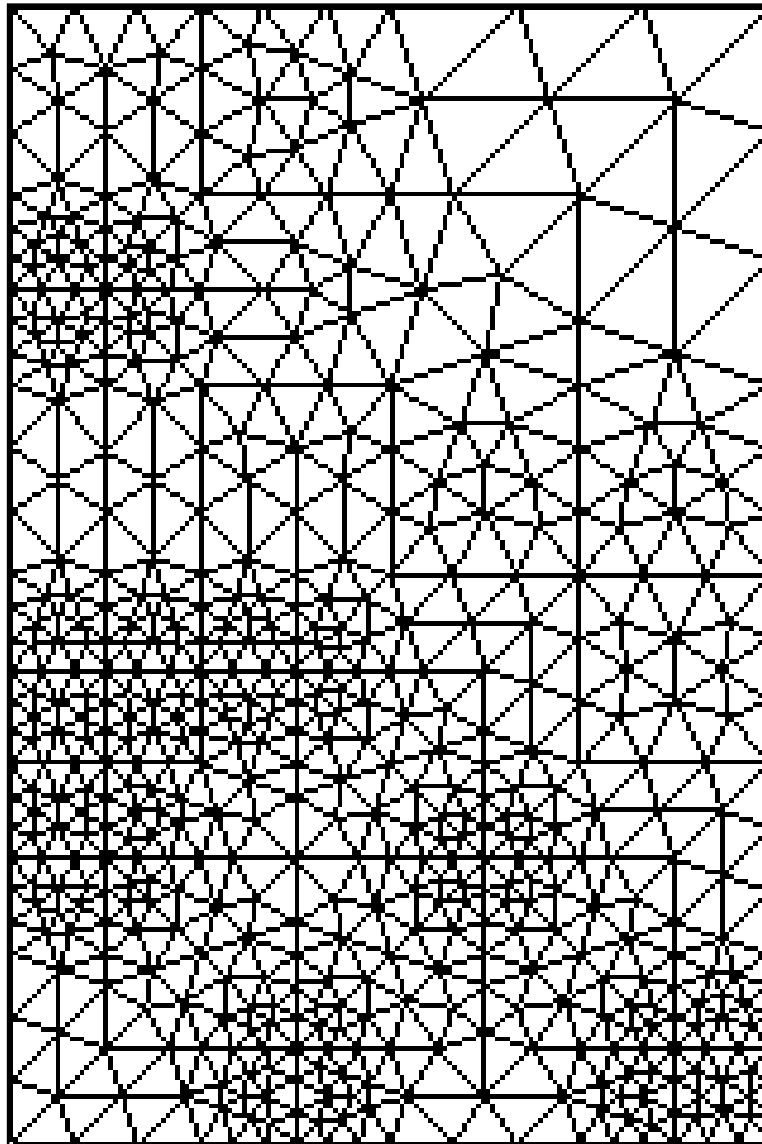
- Similar in higher dimensions

Choosing a Random Sphere

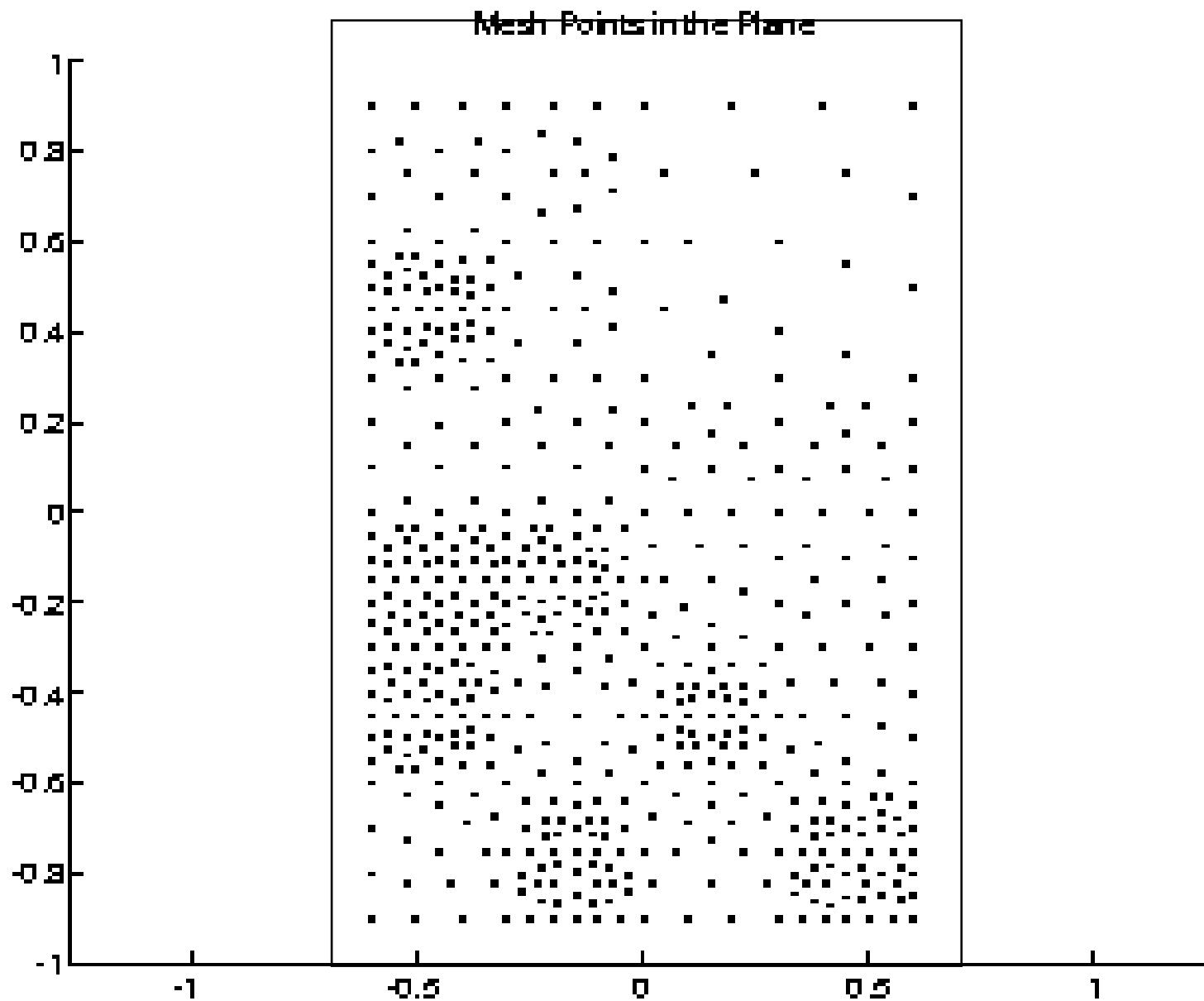
- Do stereographic projection from \mathbb{R}^d to sphere S in \mathbb{R}^{d+1}
- Find **centerpoint** of projected points
 - Any plane through centerpoint divides points ~evenly
 - There is a linear programming algorithm, cheaper heuristics
- *Conformally map* points on sphere
 - *Rotate* points around origin so centerpoint at $(0, \dots, 0, r)$ for some r
 - *Dilate* points (unproject, multiply by $((1-r)/(1+r))^{1/2}$, project)
 - this maps centerpoint to origin $(0, \dots, 0)$, spreads points around S
- Pick a random plane through origin
 - Intersection of plane and sphere S is “circle”
- Unproject circle
 - yields desired circle C in \mathbb{R}^d
- Create N_s : j belongs to N_s if $\alpha * D_j$ intersects C

Random Sphere Algorithm (Gilbert)

Finite Element Mesh



Random Sphere Algorithm (Gilbert)



Random Sphere Algorithm (Gilbert)

Points Projected onto the Sphere

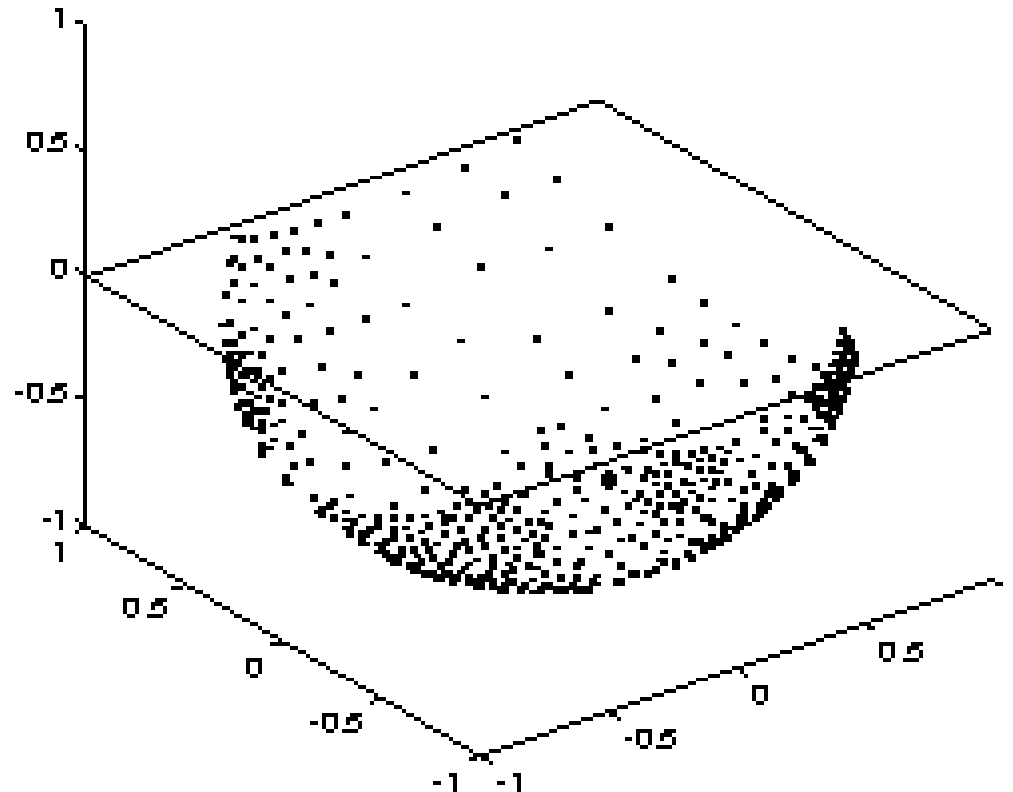
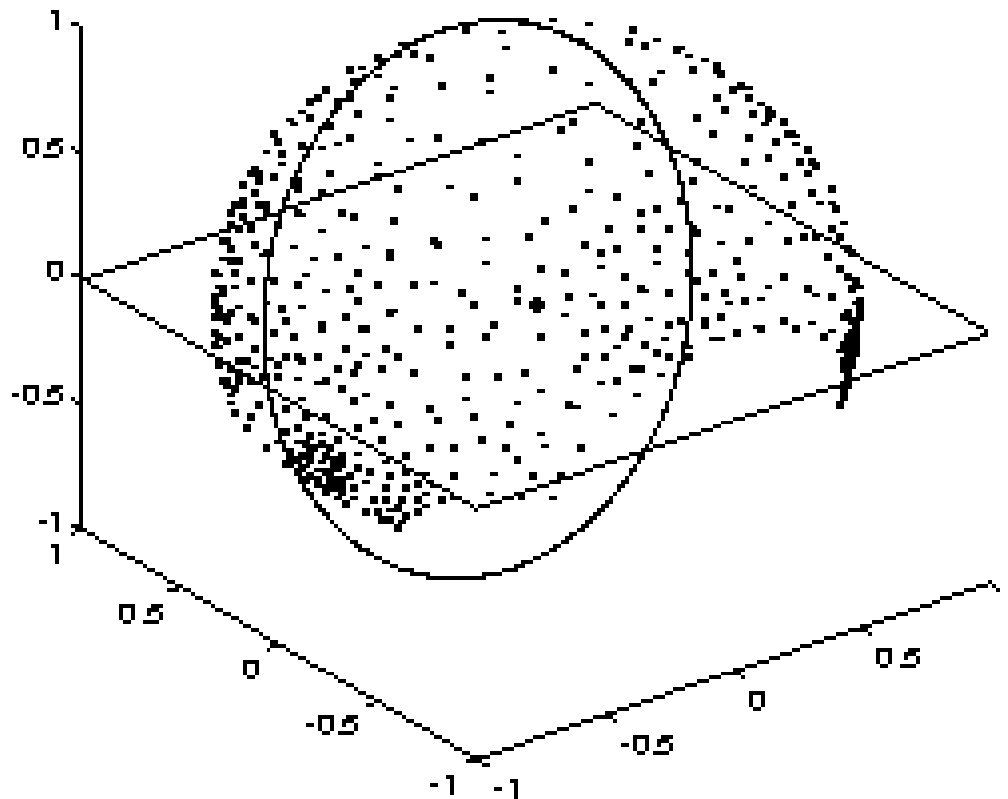


Figure 3: Projected mesh points. The large dot is the centerpoint.

Random Sphere Algorithm (Gilbert)



Random Sphere Algorithm (Gilbert)

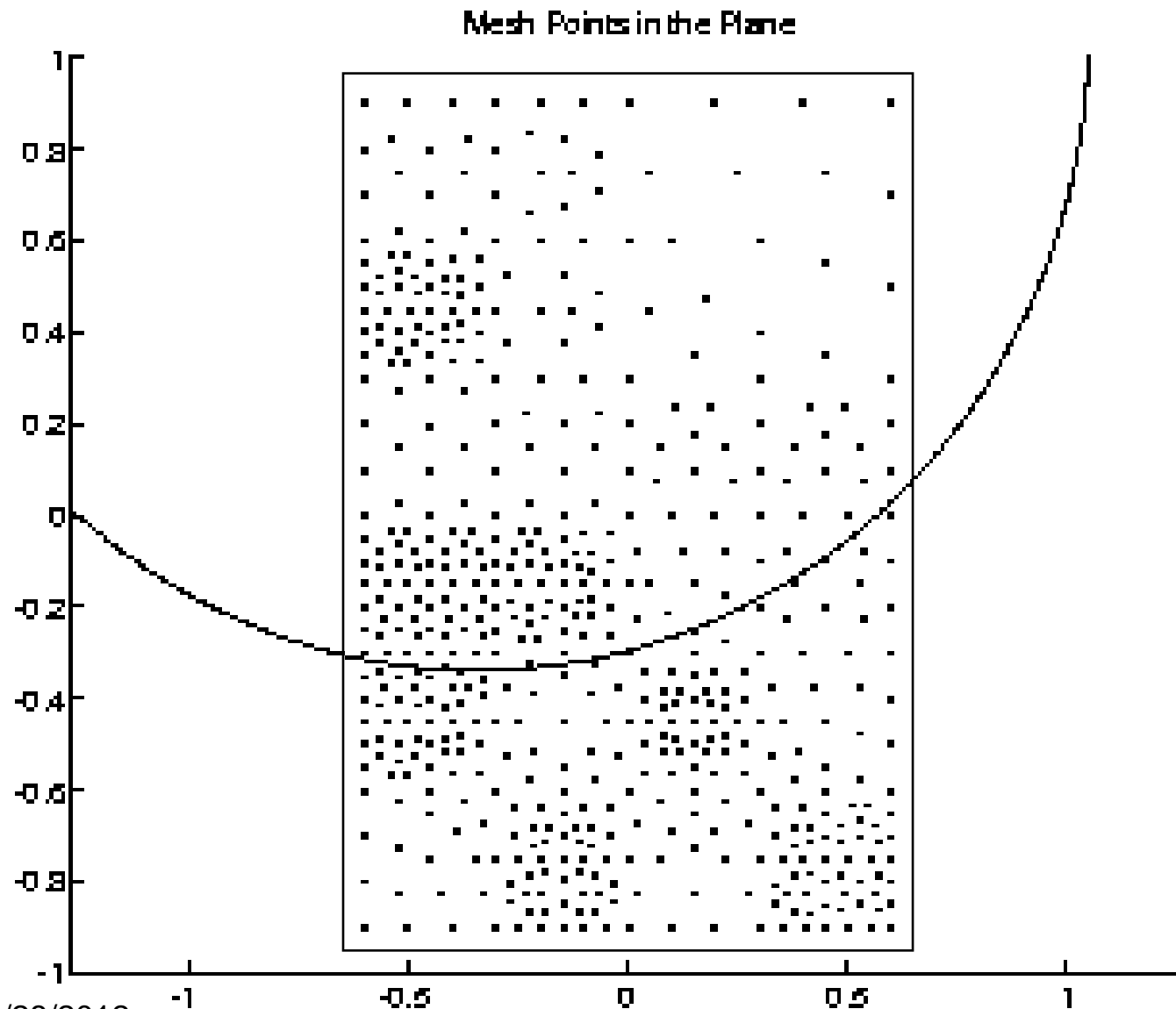
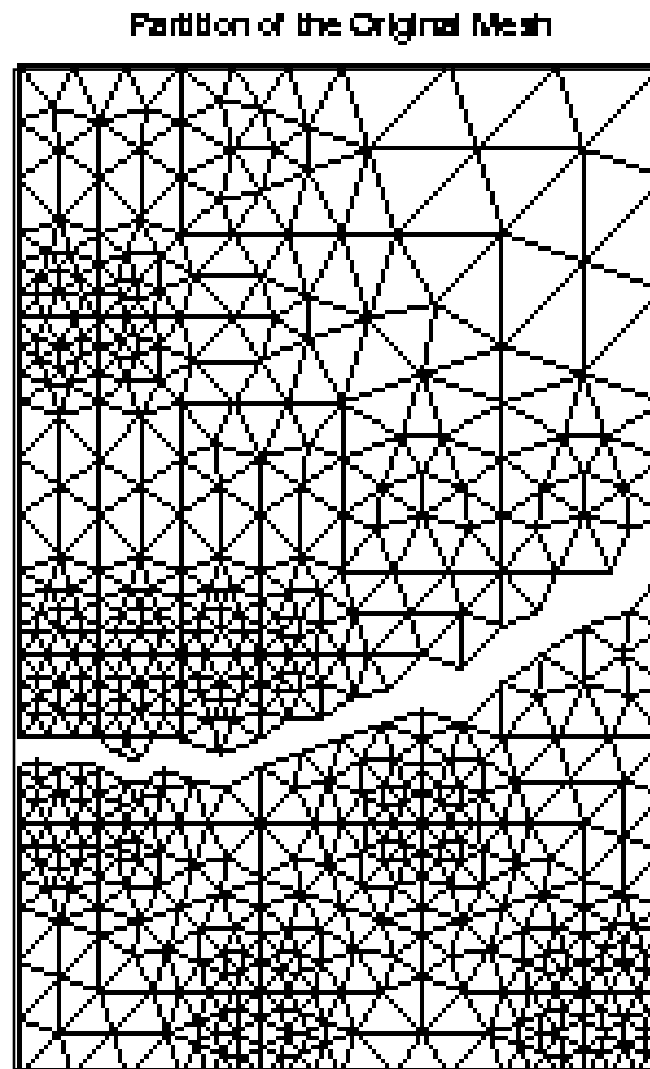
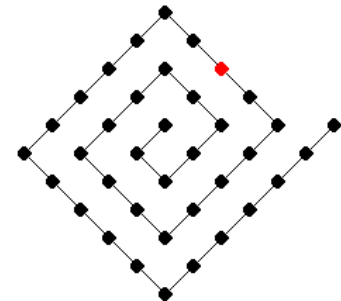


Figure 5: The separating circle projected back to the plane.



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 connection is not spatial:
-
- Details at
 - www.cs.berkeley.edu/~demmel/cs267/lecture18/lecture18.html
 - www.cs.ucsb.edu/~gilbert
 - www-bcf.usc.edu/~shanghua/



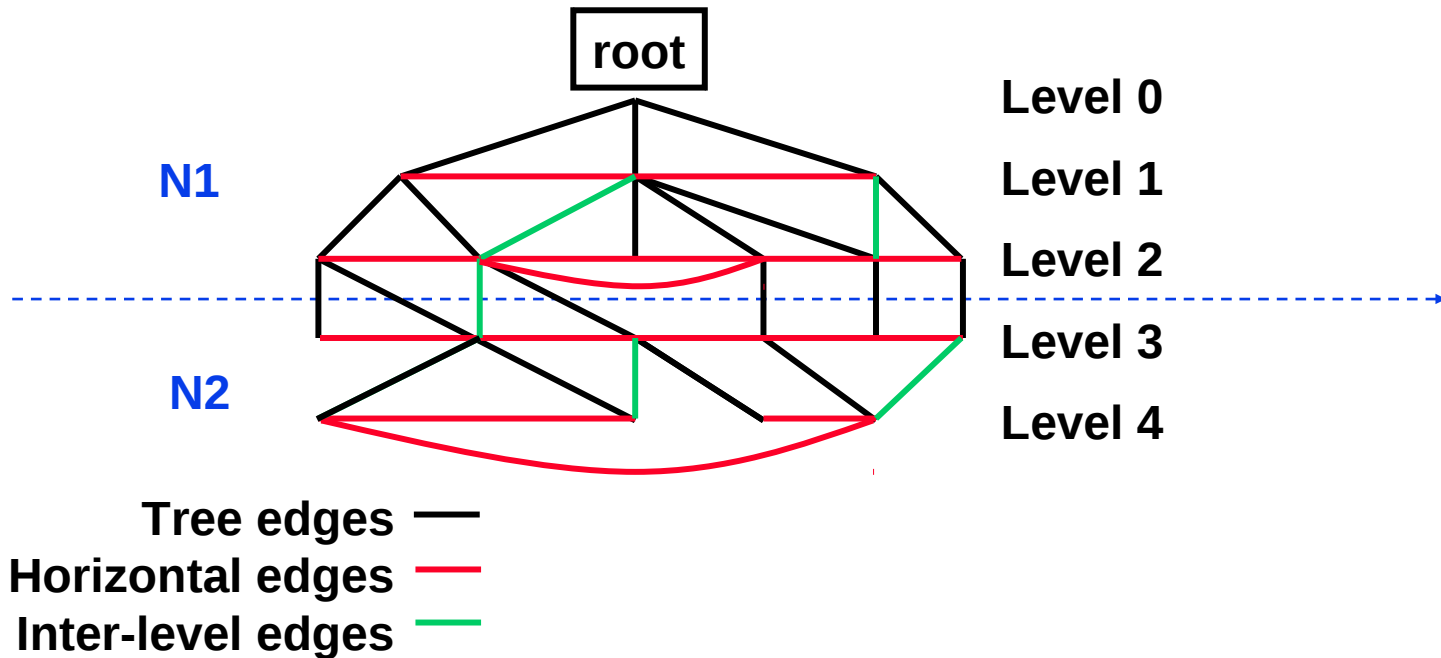
Outline of Graph Partitioning

Lectures

- 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
- Comparison of Methods and Applications
- Beyond Graph Partitioning: Hypergraphs

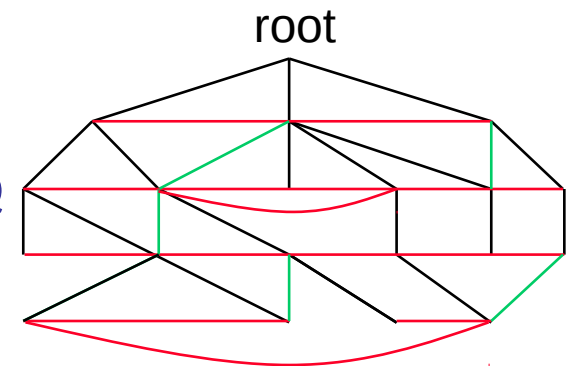
Coordinate-Free: Breadth First Search (BFS)

- Given $G(N,E)$ and a root node r in N , BFS produces
 - A subgraph T of G (same nodes, subset of edges)
 - T is a tree rooted at r
 - Each node assigned a **level** = distance from r



Breadth First Search (details)

- Queue (First In First Out, or FIFO)
 - Enqueue(x, Q) adds x to back of Q
 - $x = \text{Dequeue}(Q)$ removes x from front of Q
- Compute Tree $T(N_T, E_T)$



$N_T = \{(r, 0)\}$, $E_T = \text{empty set}$

Enqueue($(r, 0), Q$)

Mark r

While Q not empty

$(n, \text{level}) = \text{Dequeue}(Q)$

 For all unmarked children c of n

$N_T = N_T \cup (c, \text{level}+1)$

$E_T = E_T \cup (n, c)$

 Enqueue($(c, \text{level}+1), Q$)

 Mark c

 Endfor

Endwhile

... Initially $T = \text{root } r$, which is at level 0

... Put root on initially empty Queue Q

... Mark root as having been processed

... While nodes remain to be processed

... Get a node to process

... Add child c to N_T

... Add edge (n, c) to E_T

... Add child c to Q for processing

... Mark c as processed

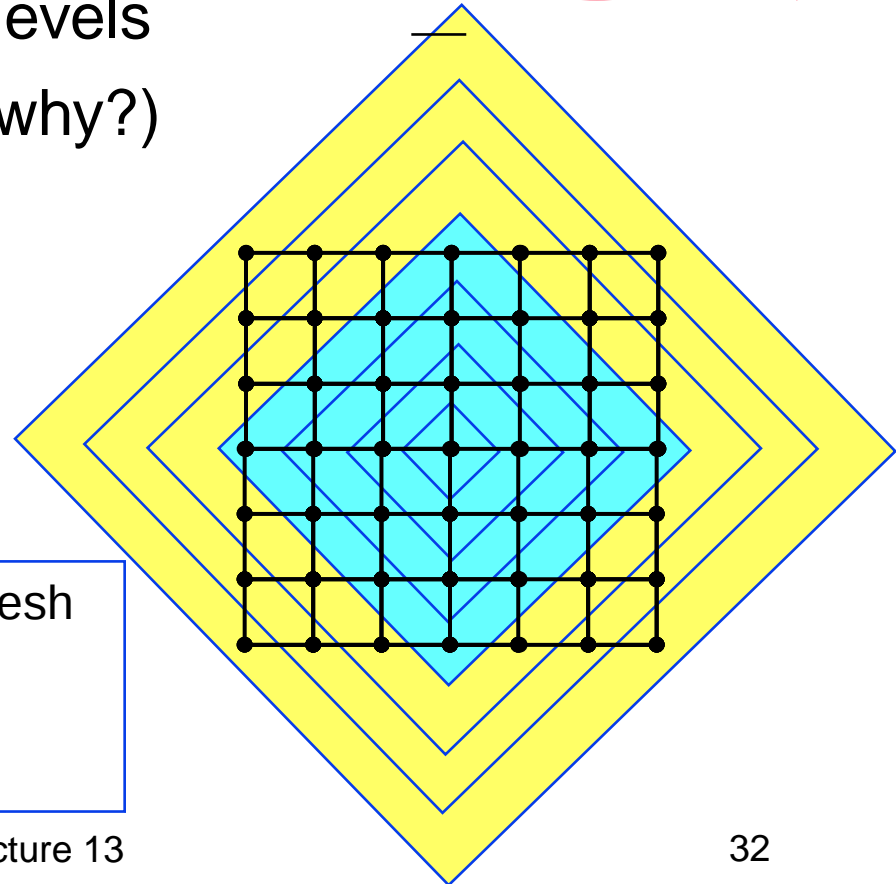
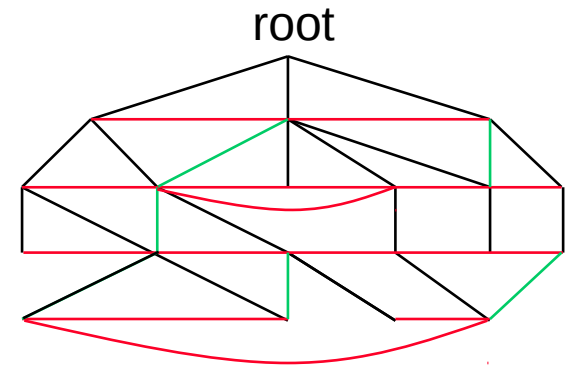
Partitioning via Breadth First Search

- BFS identifies 3 kinds of edges
 - Tree Edges - part of T
 - Horizontal Edges - connect nodes at same level
 - Interlevel Edges - connect nodes at adjacent levels
- No edges connect nodes in levels differing by more than 1 (why?)
- BFS partitioning heuristic
 - $N = N_1 \cup N_2$, where
 - $N_1 = \{\text{nodes at level } \leq L\}$,
 - $N_2 = \{\text{nodes at level } > L\}$
 - Choose L so $|N_1|$ close to $|N_2|$

BFS partition of a 2D Mesh
using center as root:

$N_1 = \text{levels } 0, 1, 2, 3$

$N_2 = \text{levels } 4, 5, 6$



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 $\text{Gain} = \sum_{k=1 \text{ to } m} \text{gain}(k)$

... 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 $\text{Gain} \leq 0$

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 $2^{-|N|/30}$

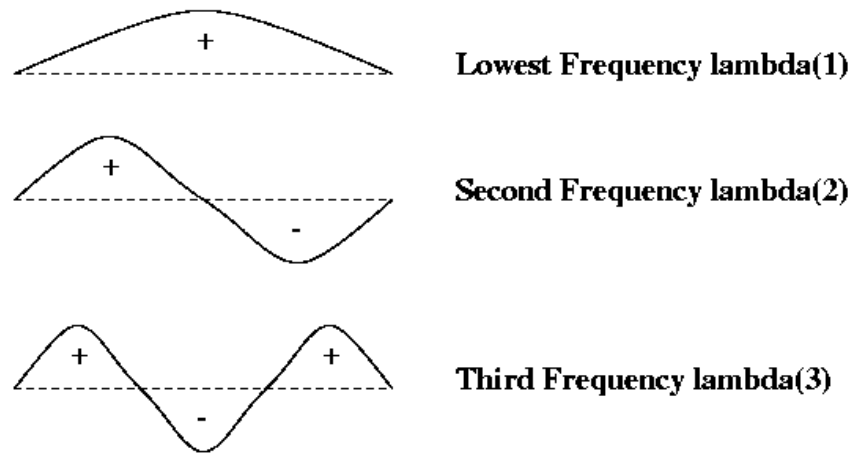
Coordinate-Free: Spectral Bisection

- 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 ~ trampoline)

Modes of a Vibrating String



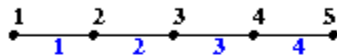
Basic Definitions

- *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

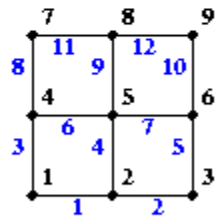


Incidence Matrix $\text{In}(G)$

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

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? First 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)

Spectral Bisection Algorithm

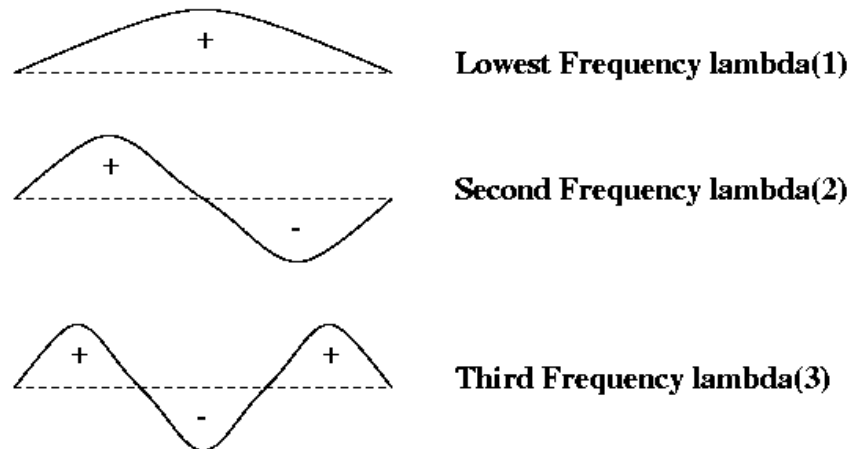
- Spectral Bisection Algorithm:
 - Compute eigenvector v_2 corresponding to $\lambda_2(L(G))$
 - For each node n of G
 - if $v_2(n) < 0$ put node n in partition N_-
 - else put node n in partition N_+
- Why does this make sense? More reasons...
 - *Theorem 4 (Fiedler, 1975):* Let G be connected, and N_1 and N_2 be any partition into part of equal size $|N|/2$. Then the number of edges connecting N_1 and N_2 is at least $.25 * |N| * \lambda_2(L(G))$.

(proof on 1996 CS267 web page)

Motivation for Spectral Bisection (recap)

- Vibrating string has **modes of vibration**, or **harmonics**
- Modes computable as follows
 - Model string as masses connected by springs (a 1D mesh)
 - Write down $F=ma$ for coupled system, get matrix A
 - Eigenvalues and eigenvectors of A are frequencies and shapes of modes
- Label nodes by whether mode - or + to get N_- and N_+
- Same idea for other graphs (eg planar graph ~ trampoline)

Modes of a Vibrating String



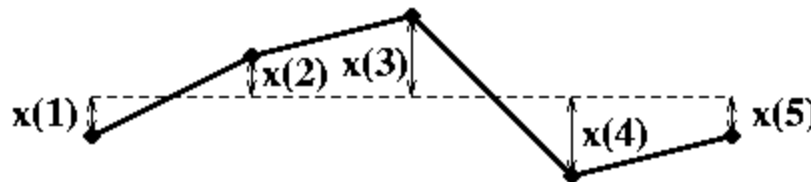
Details for Vibrating String Analogy

- Force on mass $j = k[x(j-1) - x(j)] + k[x(j+1) - x(j)]$
 $= -k[-x(j-1) + 2x(j) - x(j+1)]$
- $F=ma$ yields $m x''(j) = -k[-x(j-1) + 2x(j) - x(j+1)]$ (*)
- Writing (*) for $j=1,2,\dots,n$ yields

$$m \frac{d^2}{dx^2} \begin{pmatrix} x(1) \\ x(2) \\ \dots \\ x(j) \\ \dots \\ x(n) \end{pmatrix} = -k \begin{pmatrix} 2x(1) - x(2) \\ -x(1) + 2x(2) - x(3) \\ \dots \\ -x(j-1) + 2x(j) - x(j+1) \\ \dots \\ 2x(n-1) - x(n) \end{pmatrix} = -k \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & \dots & \dots & \\ & & -1 & 2 & -1 \\ & & & \dots & \dots \\ & & & & -1 & 2 \end{pmatrix} \begin{pmatrix} x(1) \\ x(2) \\ \dots \\ x(j) \\ \dots \\ x(n) \end{pmatrix} = -k L \begin{pmatrix} x(1) \\ x(2) \\ \dots \\ x(j) \\ \dots \\ x(n) \end{pmatrix}$$

$$(-m/k) x'' = L x$$

Vibrating Mass Spring System



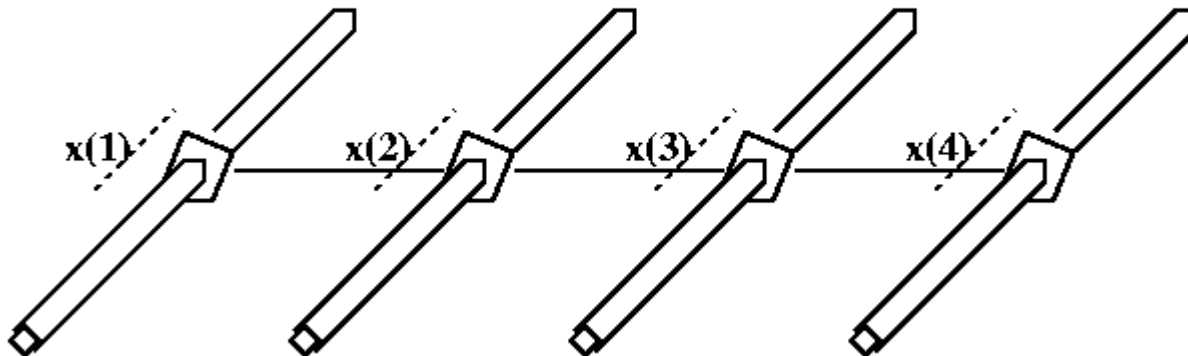
Details for Vibrating String (continued)

- $-(m/k) x'' = L^*x$, where $x = [x_1, x_2, \dots, x_n]^T$
- Seek solution of form $x(t) = \sin(\alpha^*t) * x_0$
 - $L^*x_0 = (m/k)^*\alpha^2 * x_0 = \lambda * x_0$
 - For each integer i , get $\lambda = 2*(1-\cos(i*\pi/(n+1)))$, $x_0 = \begin{pmatrix} \sin(1*i*\pi/(n+1)) \\ \sin(2*i*\pi/(n+1)) \\ \dots \\ \sin(n*i*\pi/(n+1)) \end{pmatrix}$
 - Thus x_0 is a sine curve with frequency proportional to i
 - Thus $\alpha^2 = 2*k/m *(1-\cos(i*\pi/(n+1)))$ or $\alpha \sim (k/m)^{1/2} * \pi * i/(n+1)$
- $L = \begin{pmatrix} 2 & -1 & & \\ -1 & 2 & -1 & \\ & \dots & \dots & \\ & & -1 & 2 \end{pmatrix}$ not quite Laplacian of 1D mesh,
but we can fix that ...

Motivation for Spectral Bisection

- Vibrating string has **modes of vibration**, or **harmonics**
- Modes computable as follows
 - Model string as masses connected by springs (a 1D mesh)
 - Write down $F=ma$ for coupled system, get matrix A
 - Eigenvalues and eigenvectors of A are frequencies and shapes of modes
- Label nodes by whether mode - or + to get N_- and N_+
- Same idea for other graphs (eg planar graph ~ trampoline)

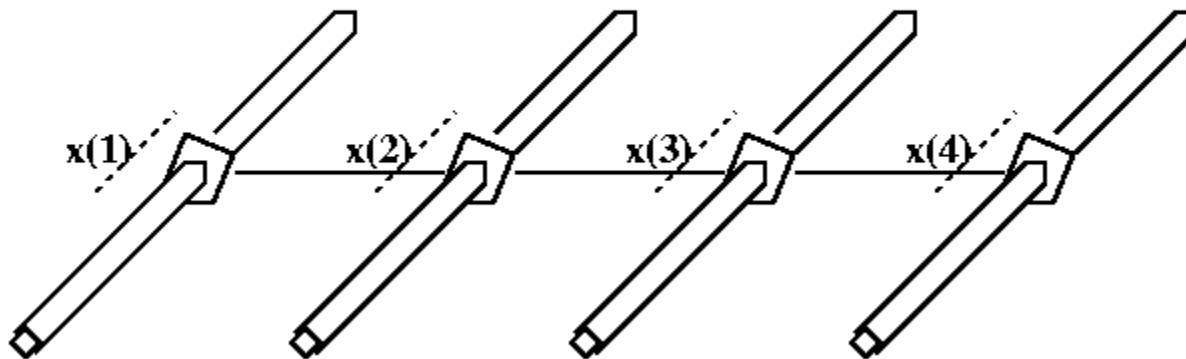
"Vibrating String" for Spectral Bisection



Details for Vibrating String (continued)

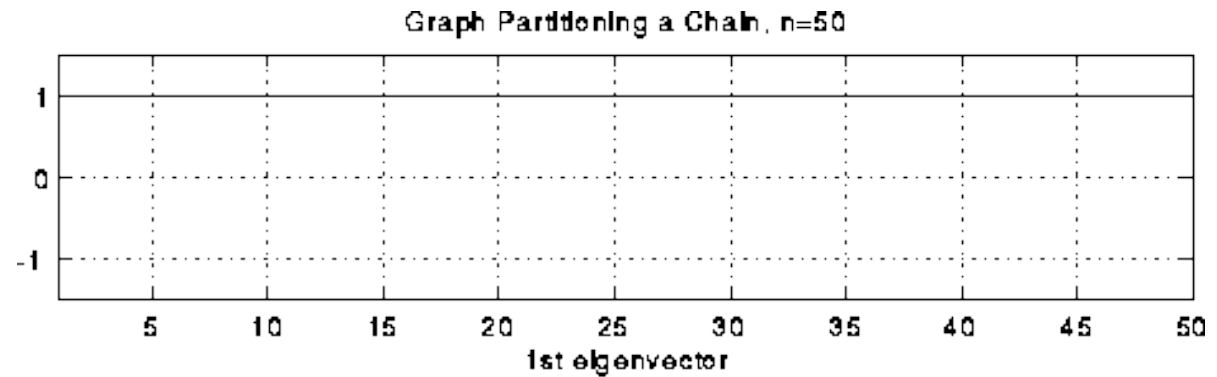
- Write down $F=ma$ for “vibrating string” below
- Get Graph Laplacian of 1D mesh

"Vibrating String" for Spectral Bisection

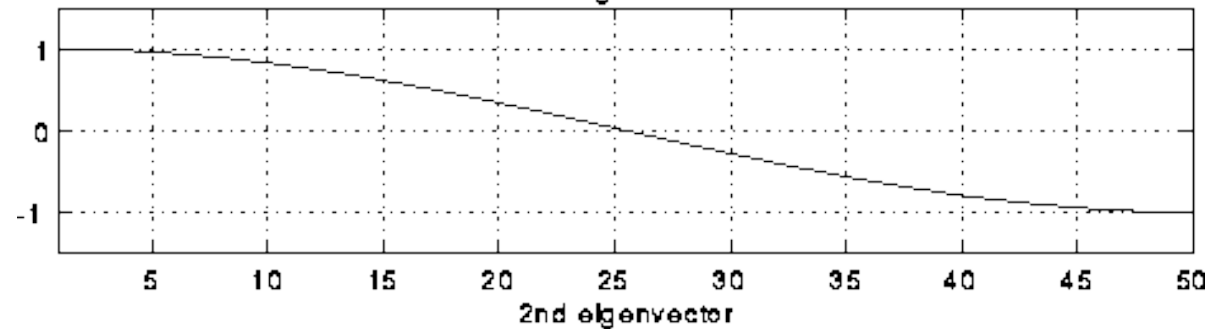


Eigenvectors of L(1D mesh)

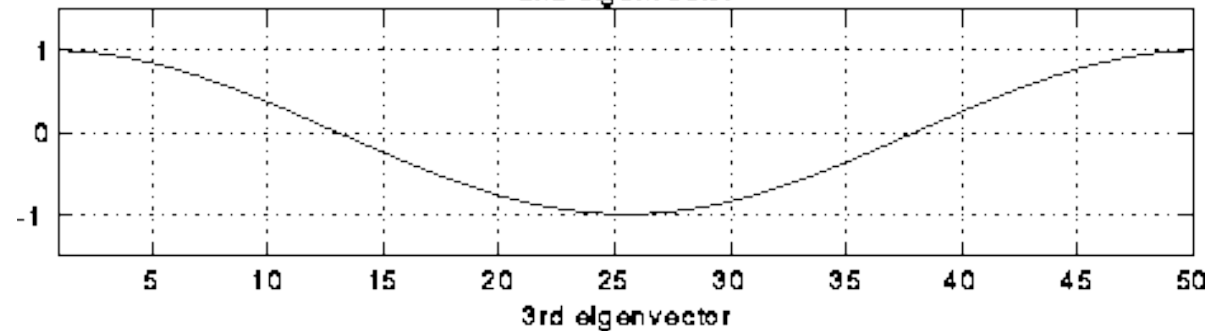
Eigenvector 1
(all ones)



Eigenvector 2

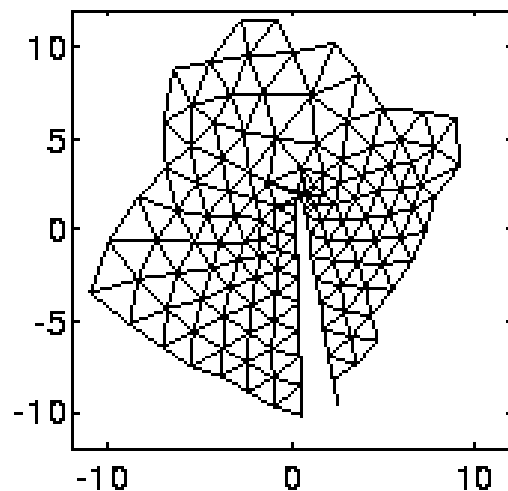


Eigenvector 3

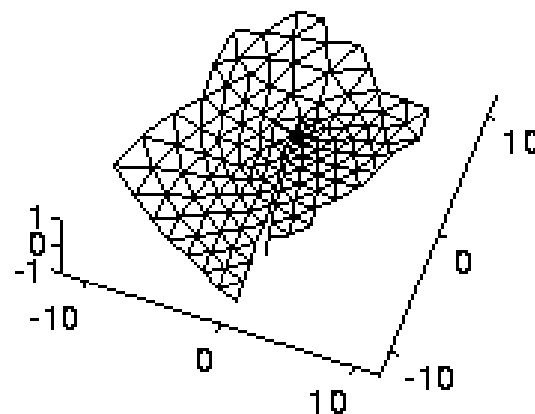


2nd eigenvector of L (planar mesh)

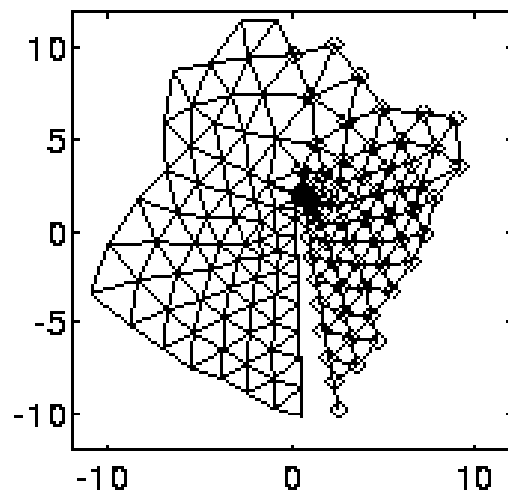
Original FE mesh



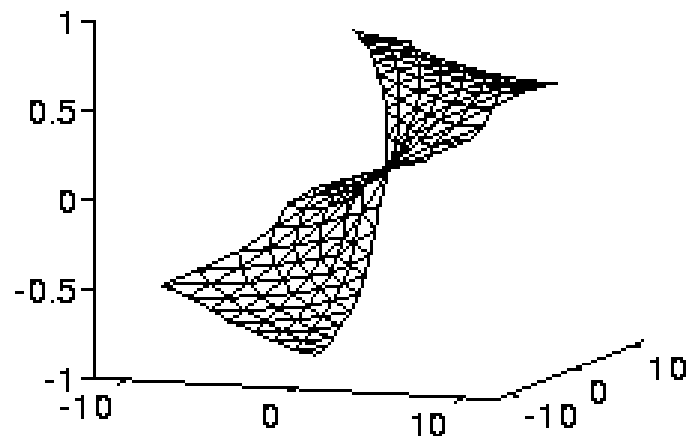
Plot of v_2 from above



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

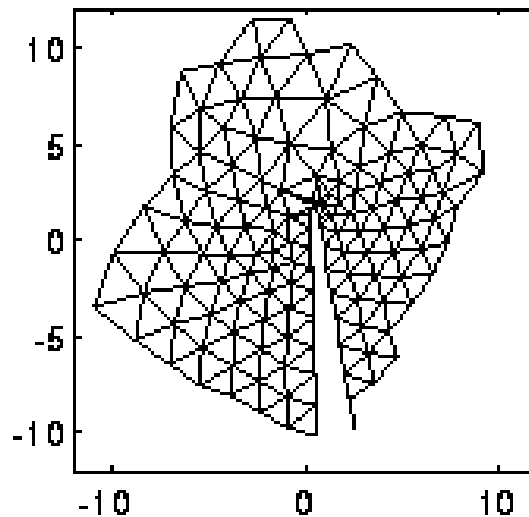


Plot of v_2 head on

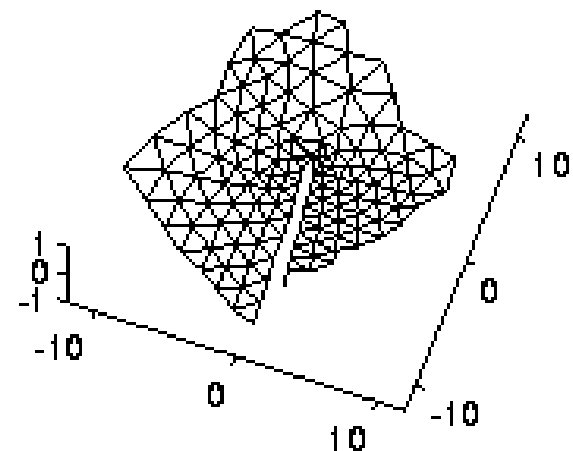


4th eigenvector of L (planar mesh)

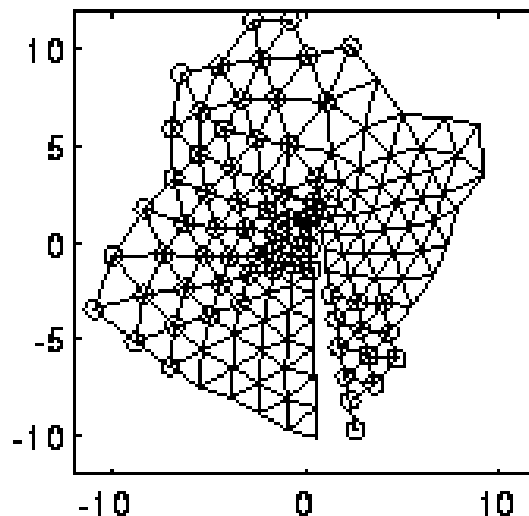
Original FE mesh



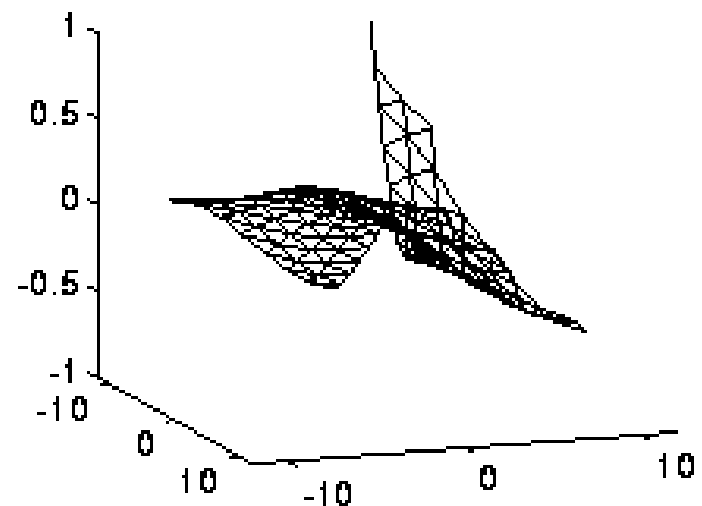
Plot of v_4 from above



Circle node i if $v_4(i) > 0$



Plot of v_4 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

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

- 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
- 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
- Comparison of Methods and Applications
- 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

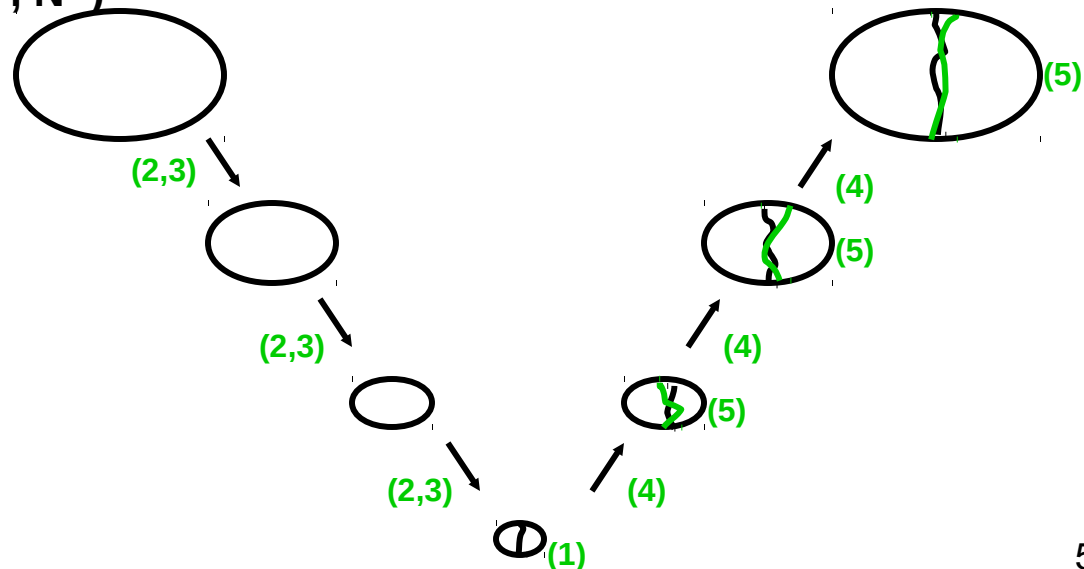
(5) Improve the partition (N^+, N^-)

Return (N^+, N^-)

endif

“V - cycle:”

How do we
Coarsen?
Expand?
Improve?



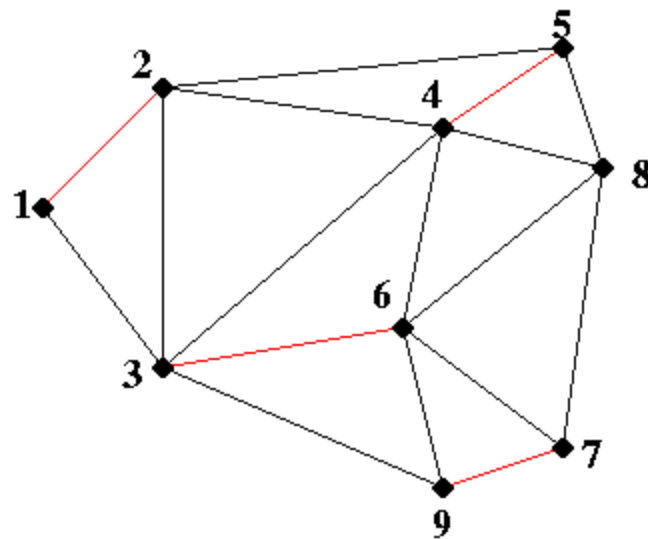
Multilevel Kernighan-Lin

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

Maximal Matching

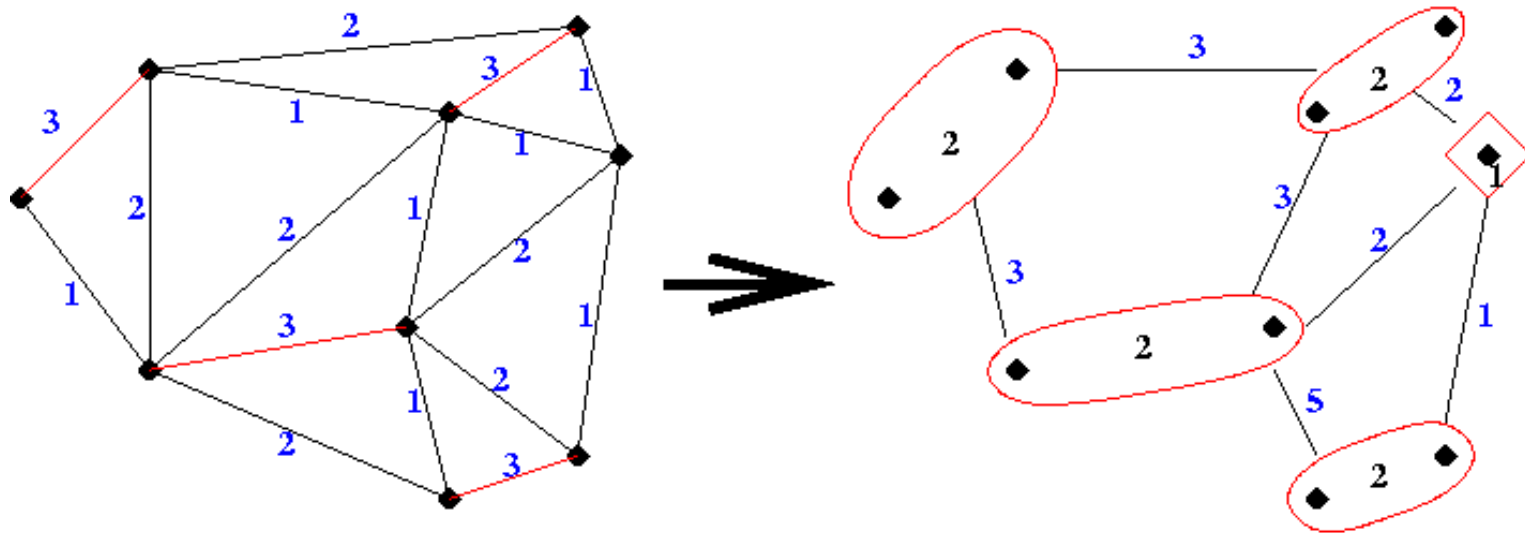
- *Definition:* A **matching** of a graph $G(N,E)$ is a subset E_m of E such that no two edges in E_m share an endpoint
- *Definition:* A **maximal matching** of a graph $G(N,E)$ is a matching E_m to which no more edges can be added and remain a matching
- A simple greedy algorithm computes a maximal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

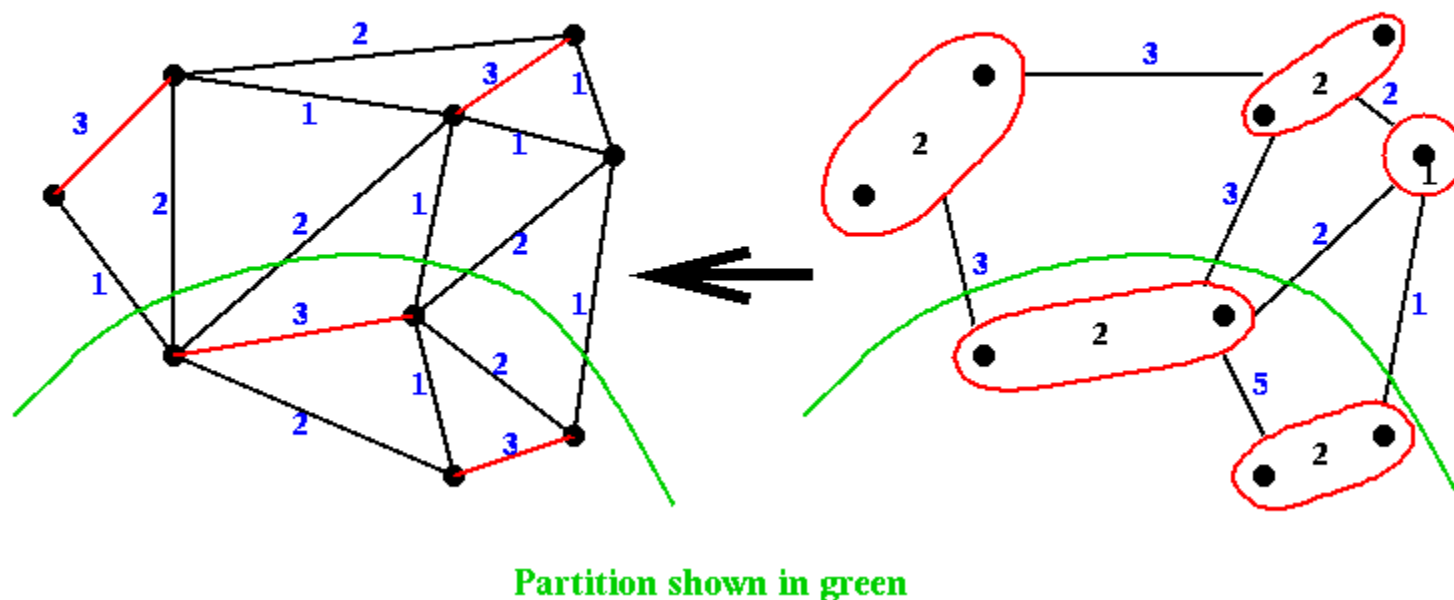
$W(ee) = W(e')$

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

adding edge weights

Expanding a partition of G_c to a partition of G

Converting a coarse partition to a fine partition



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** 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
  
```

Maximal Independent Subset N_i of N

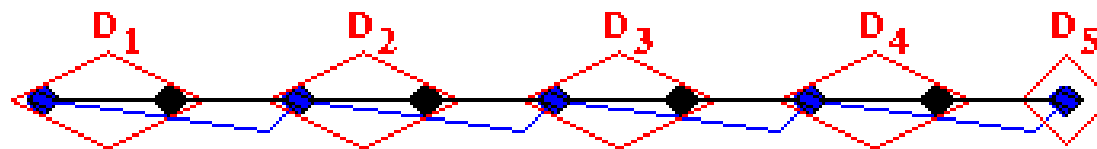


◆ and ◆ - nodes of N

◆ - nodes of N_i

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

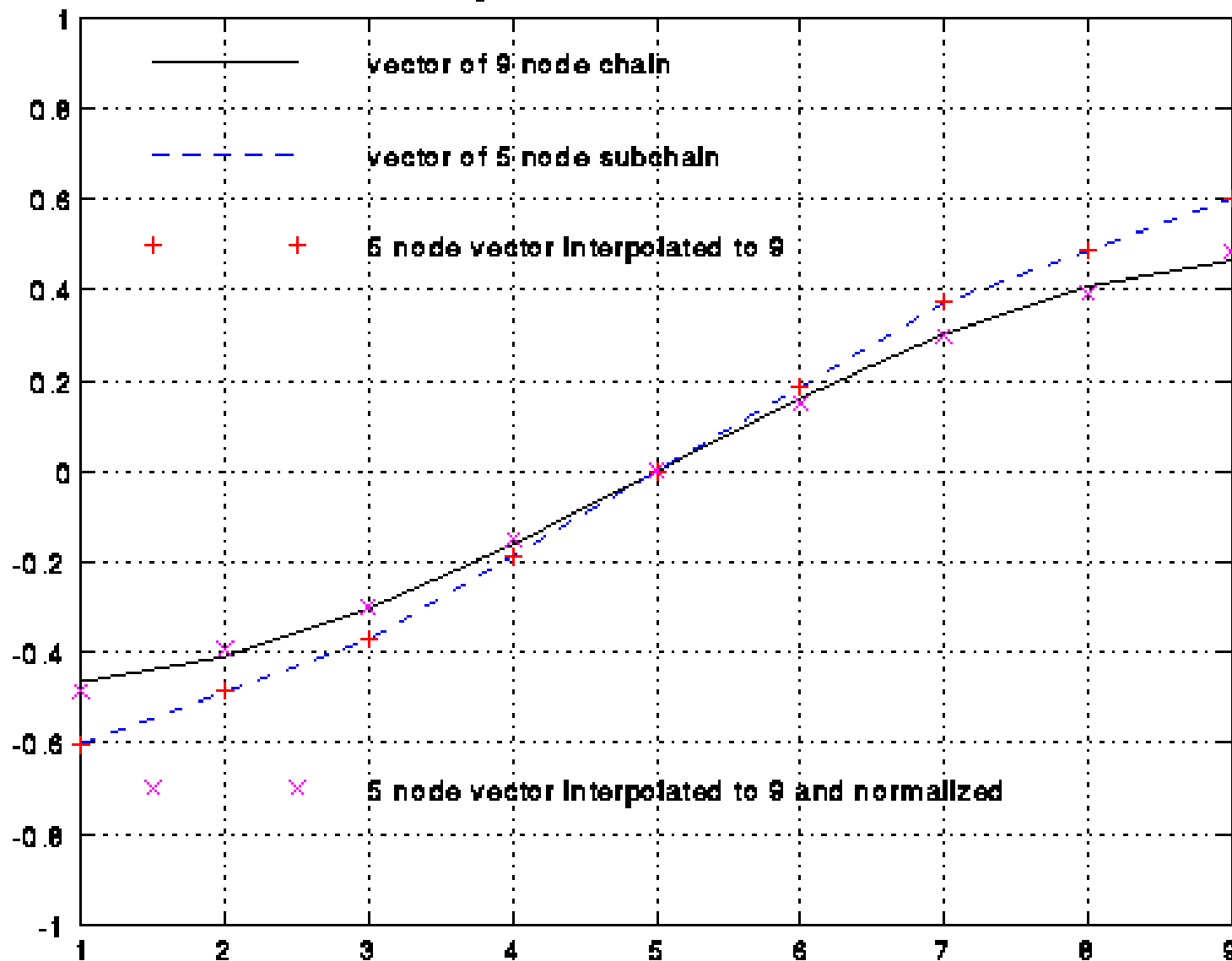
until no unmarked edges

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

2nd Eigenvectors of G = chain of 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,

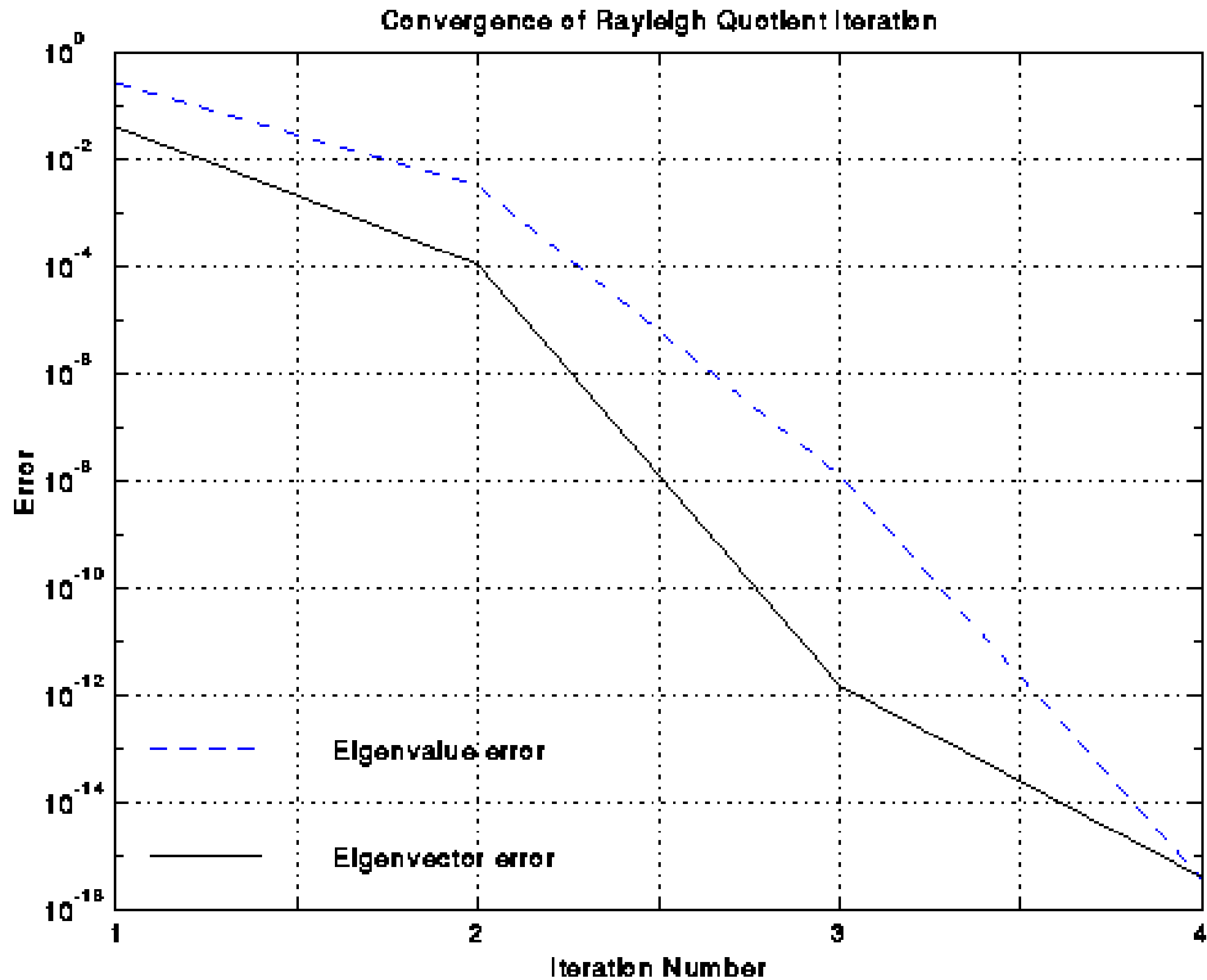
... which uses matrix-vector multiply (no surprise)

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

until $v(j)$ converges

... Convergence is very fast: cubic

Example of convergence for 1D mesh



Outline of Graph Partitioning

Lectures

- 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
- **Comparison of Methods and Applications**
- Beyond Graph Partitioning: Hypergraphs

Available Implementations

- **Multilevel Kernighan/Lin**
 - METIS (www.cs.umn.edu/~metis)
 - ParMETIS - parallel version
- **Multilevel Spectral Bisection**
 - S. Barnard and H. Simon, “A fast multilevel implementation of recursive spectral bisection ...”, Proc. 6th SIAM Conf. On Parallel Processing, 1993
 - Chaco (www.cs.sandia.gov/CRF/papers_chaco.html)
- **Hybrids possible**
 - Ex: Using Kernighan/Lin to improve a partition from spectral bisection
- **Recent package, collection of techniques**
 - Zoltan (www.cs.sandia.gov/Zoltan)
- **See www.cs.sandia.gov/~bahendr/partitioning.html**

Comparison of methods

- Compare only methods that use edges, not nodal coordinates
 - CS267 webpage and KK95a (see below) have other comparisons
- Metrics
 - Speed of partitioning
 - Number of edge cuts
 - Other application dependent metrics
- Summary
 - No one method best
 - Multi-level Kernighan/Lin fastest by far, comparable to Spectral in the number of edge cuts
 - www-users.cs.umn.edu/~karypis/metis/publications/main.html
 - see publications KK95a and KK95b
 - Spectral give much better cuts for some applications
 - Ex: image segmentation
 - See “Normalized Cuts and Image Segmentation” by J. Malik, J. Shi

Number of edges cut for a 64-way partition

For Multilevel Kernighan/Lin, as implemented in [METIS](#) (see KK95a)

Graph	# of Nodes	# of Edges	# Edges cut for 64-way partition	Expected # cuts for 2D mesh	Expected # cuts for 3D mesh	Description
144	144649	1074393	88806	6427	31805	3D FE Mesh
4ELT	15606	45878	2965	2111	7208	2D FE Mesh
ADD32	4960	9462	675	1190	3357	32 bit adder
AUTO	448695	3314611	194436	11320	67647	3D FE Mesh
BBMAT	38744	993481	55753	3326	13215	2D Stiffness M.
FINAN512	74752	261120	11388	4620	20481	Lin. Prog.
LHR10	10672	209093	58784	1746	5595	Chem. Eng.
MAP1	267241	334931	1388	8736	47887	Highway Net.
MEMPLUS	17758	54196	17894	2252	7856	Memory circuit
SHYY161	76480	152002	4365	4674	20796	Navier-Stokes
TORSO	201142	1479989	117997	7579	39623	3D FE Mesh

Expected # cuts for 64-way partition of 2D mesh of n nodes

$$n^{1/2} + 2*(n/2)^{1/2} + 4*(n/4)^{1/2} + \dots + 32*(n/32)^{1/2} \sim 17 * n^{1/2}$$

Expected # cuts for 64-way partition of 3D mesh of n nodes =

$$n^{2/3} + 2*(n/2)^{2/3} + 4*(n/4)^{2/3} + \dots + 32*(n/32)^{2/3} \sim 11.5 * n^{2/3}$$

Speed of 256-way partitioning (from KK95a)

Partitioning time in seconds

Graph	# of Nodes	# of Edges	Multilevel Spectral Bisection	Multilevel Kernighan/Lin	Description
144	144649	1074393	607.3	48.1	3D FE Mesh
4ELT	15606	45878	25.0	3.1	2D FE Mesh
ADD32	4960	9462	18.7	1.6	32 bit adder
AUTO	448695	3314611	2214.2	179.2	3D FE Mesh
BBMAT	38744	993481	474.2	25.5	2D Stiffness M.
FINAN512	74752	261120	311.0	18.0	Lin. Prog.
LHR10	10672	209093	142.6	8.1	Chem. Eng.
MAP1	267241	334931	850.2	44.8	Highway Net.
MEMPLUS	17758	54196	117.9	4.3	Memory circuit
SHYY161	76480	152002	130.0	10.1	Navier-Stokes
TORSO	201142	1479989	1053.4	63.9	3D FE Mesh

Kernighan/Lin much faster than Spectral Bisection!

Outline of Graph Partitioning

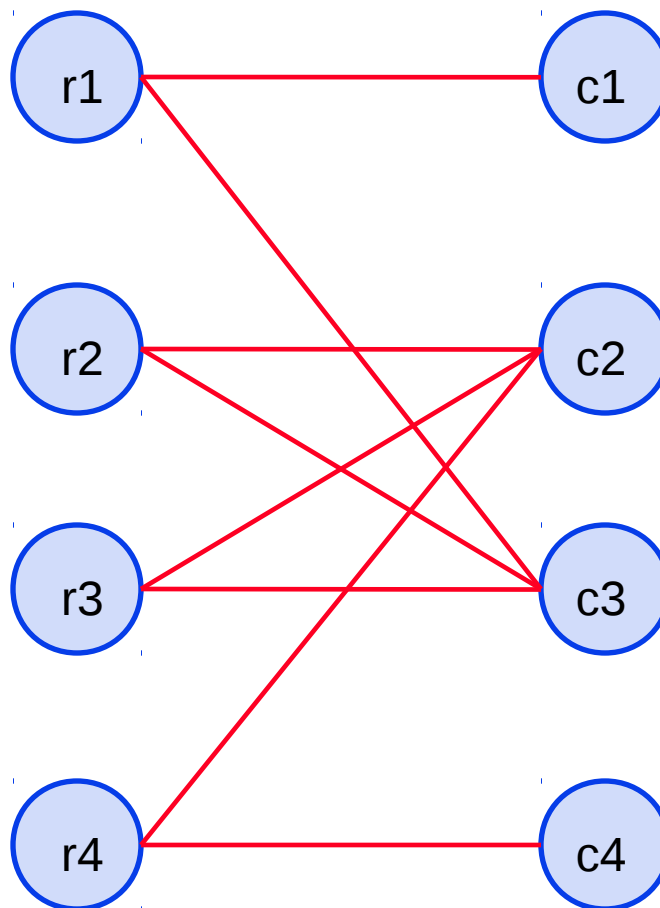
Lectures

- 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
- Comparison of Methods and Applications
- **Beyond Graph Partitioning: Hypergraphs**

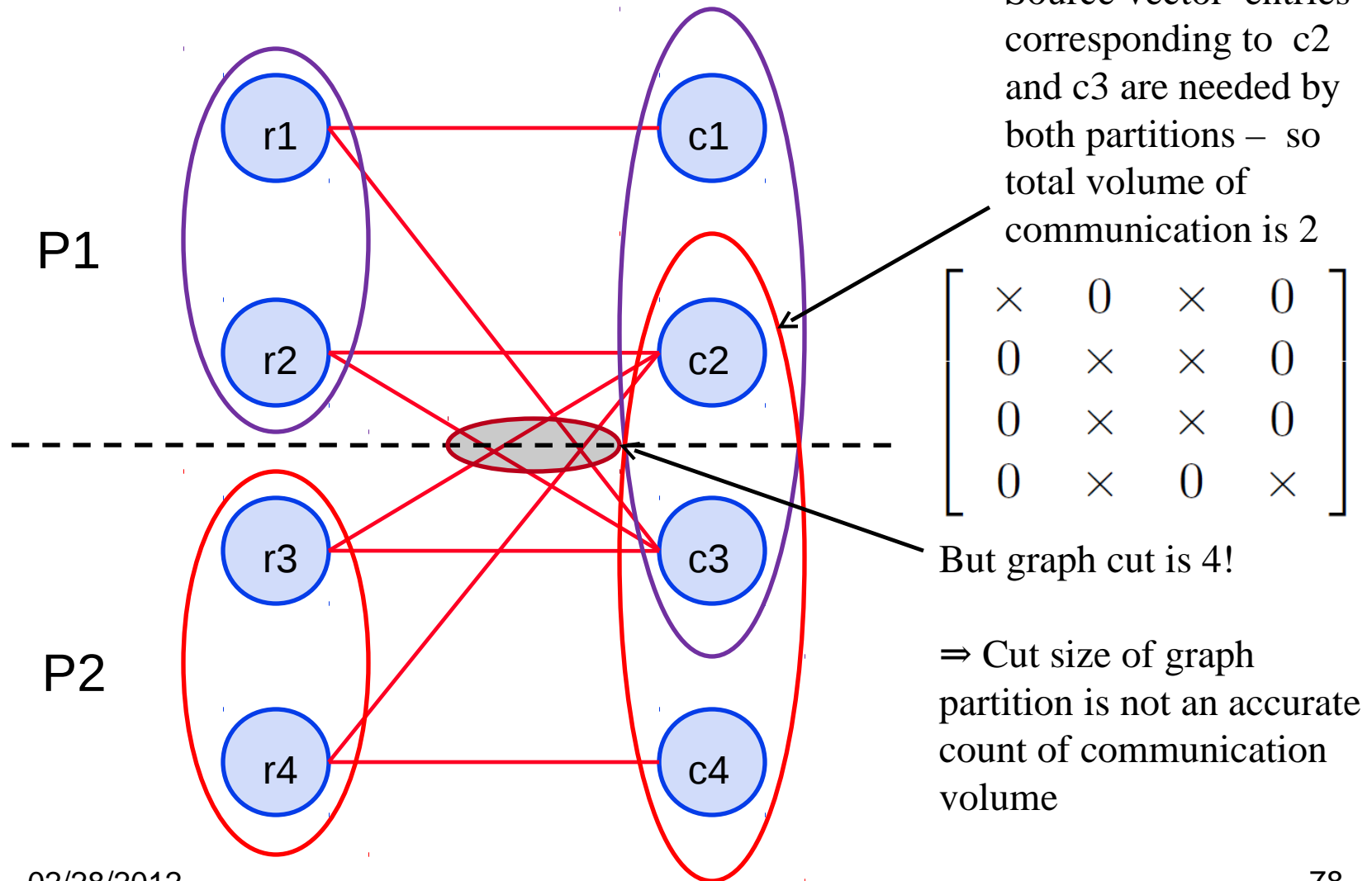
Beyond simple graph partitioning:

Representing a sparse matrix as a hypergraph

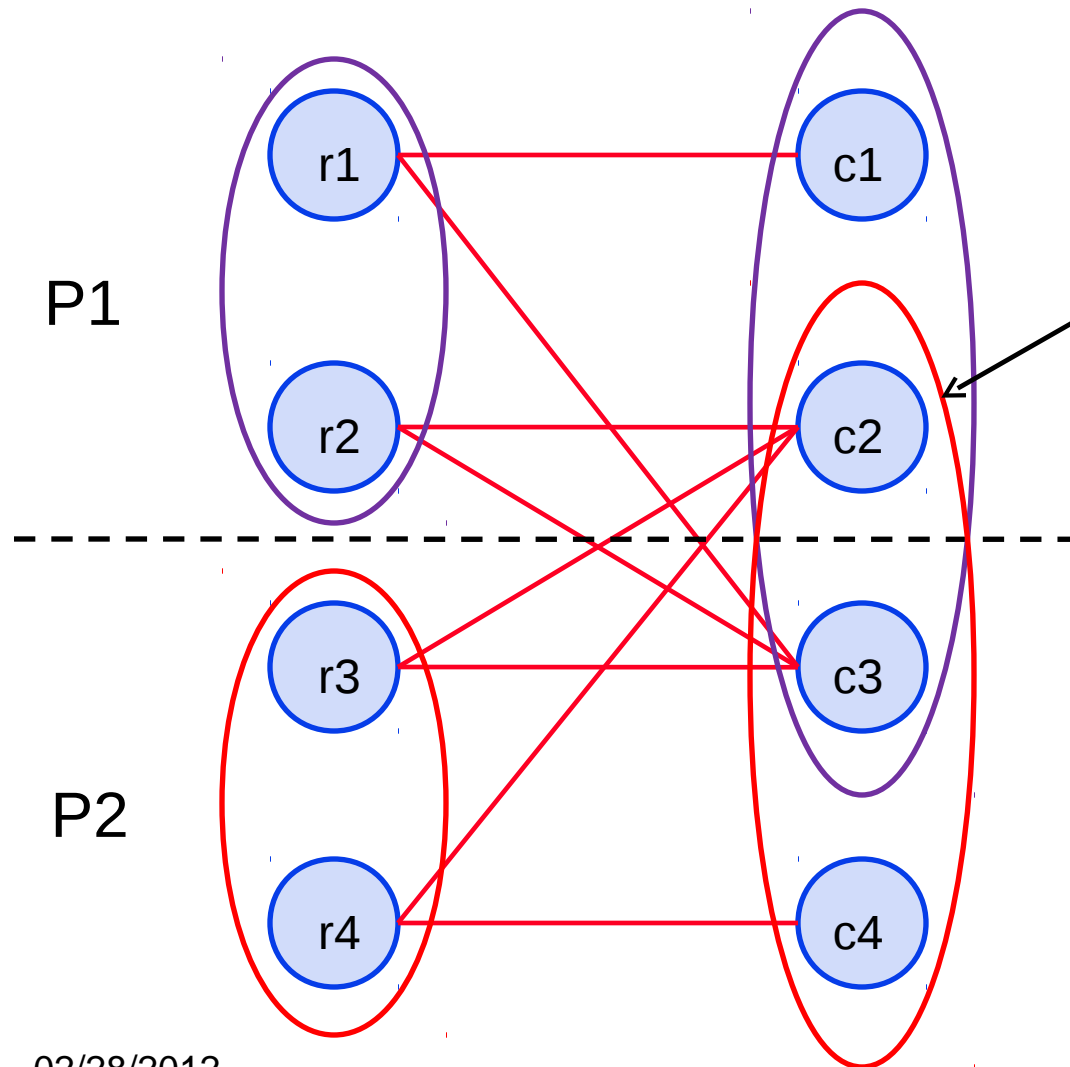
$$\begin{bmatrix} \times & 0 & \times & 0 \\ 0 & \times & \times & 0 \\ 0 & \times & \times & 0 \\ 0 & \times & 0 & \times \end{bmatrix}$$



Using a graph to partition, versus a hypergraph



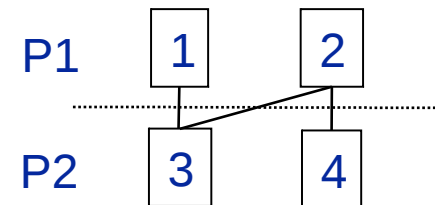
Using a graph to partition, versus a hypergraph



Source vector entries corresponding to c_2 and c_3 are needed by both partitions – so total volume of communication is 2

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

But graph cut is 3!

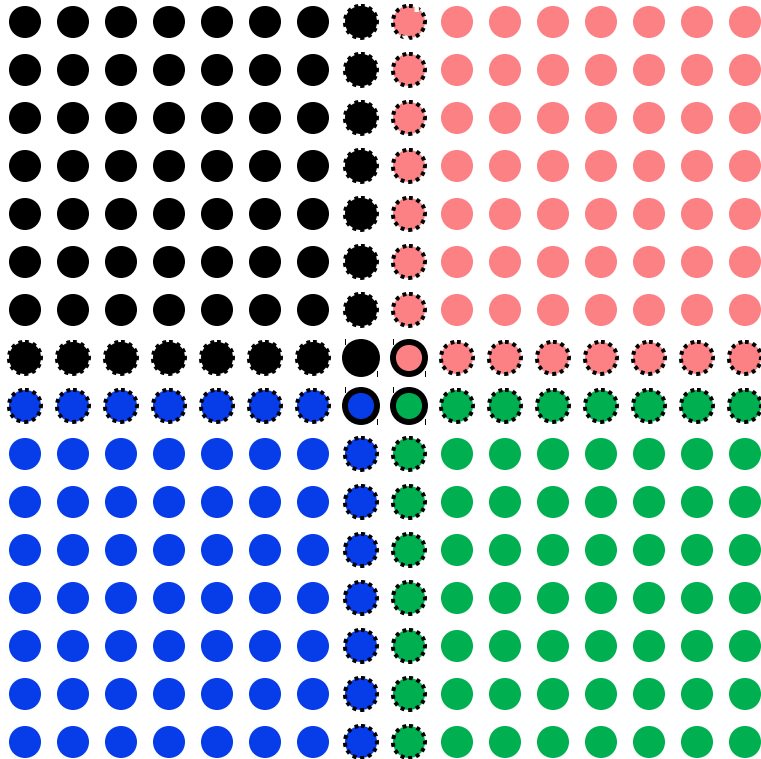


⇒ Cut size of graph partition may not accurately count communication volume

Two Different 2D Mesh Partitioning Strategies

Graph:

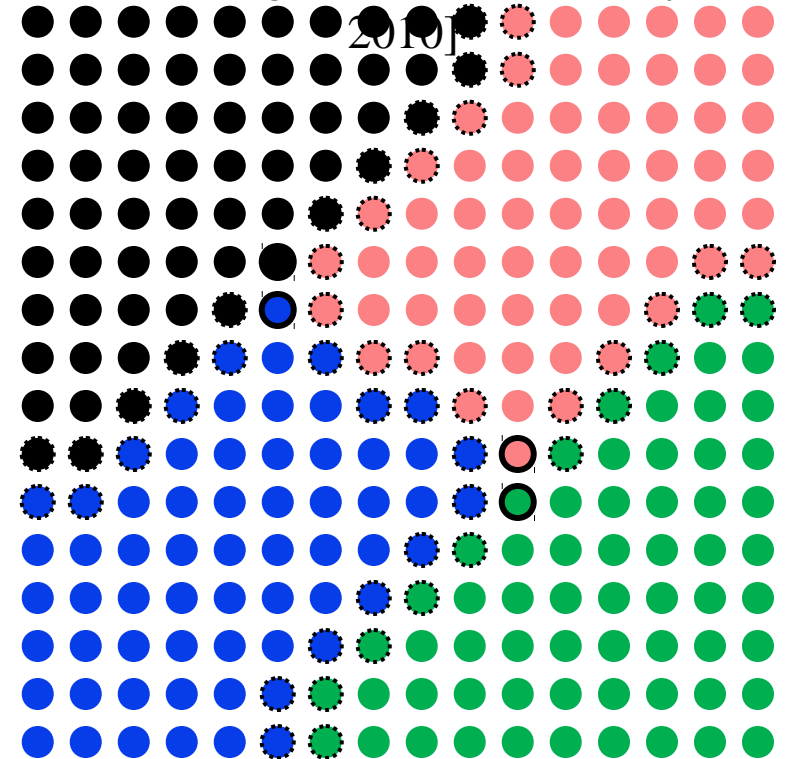
Cartesian Partitioning



Total SpMV communication volume = 64

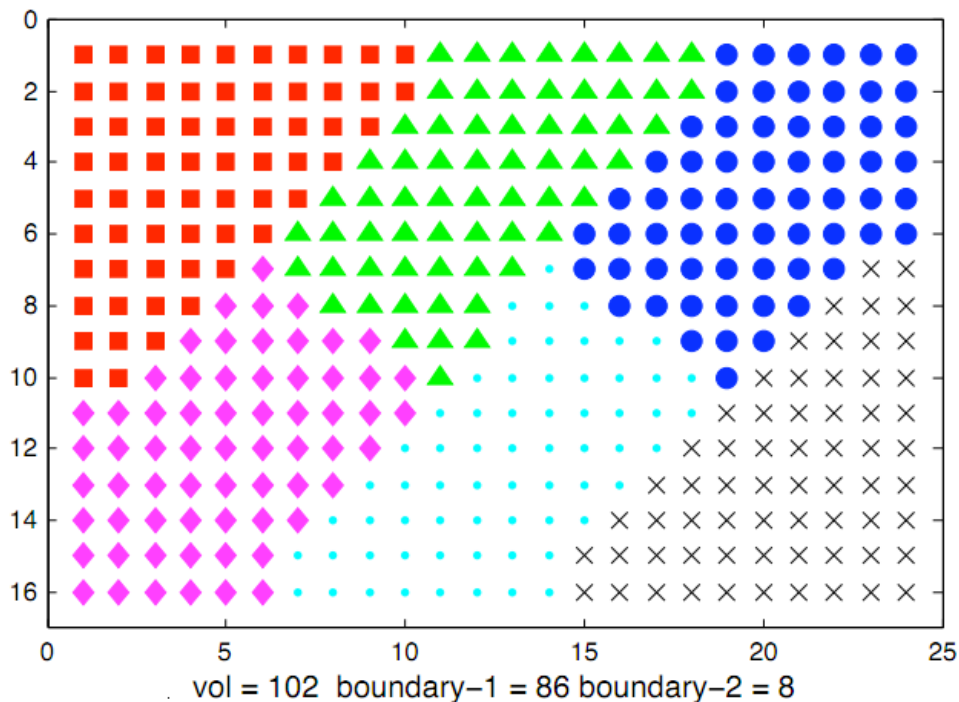
Hypergraph:

MeshPart Algorithm [Ucar, Catalyurek, 2010]

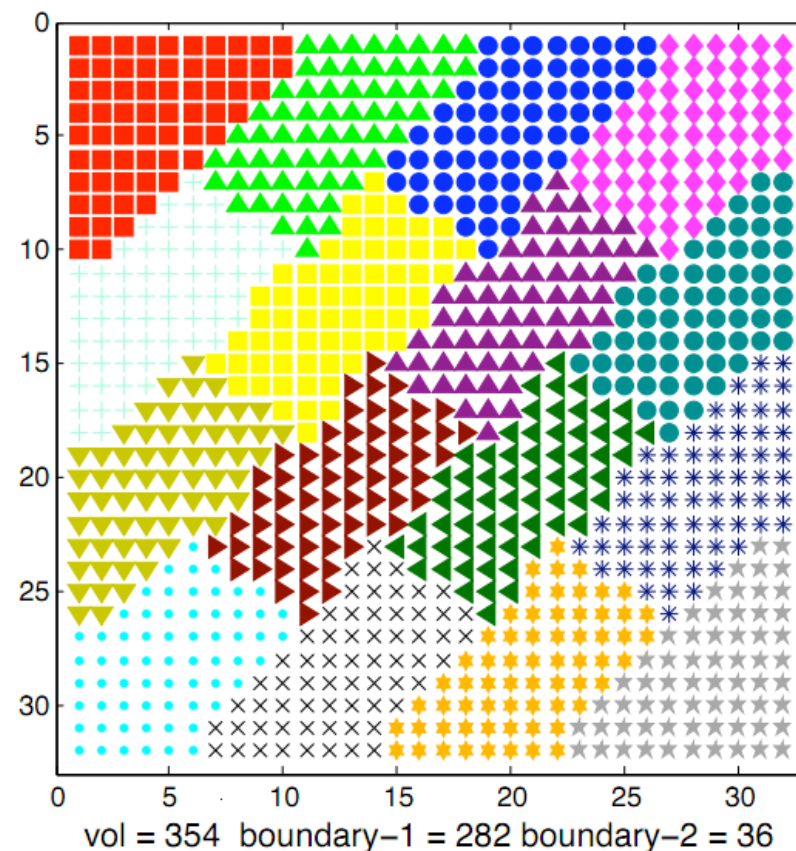


Total SpMV communication volume = 58

Generalization of the MeshPart Algorithm



(a) 2×3 -way partitioning of the 16×24 mesh



(c) 16-way partitioning of the 32×32 mesh

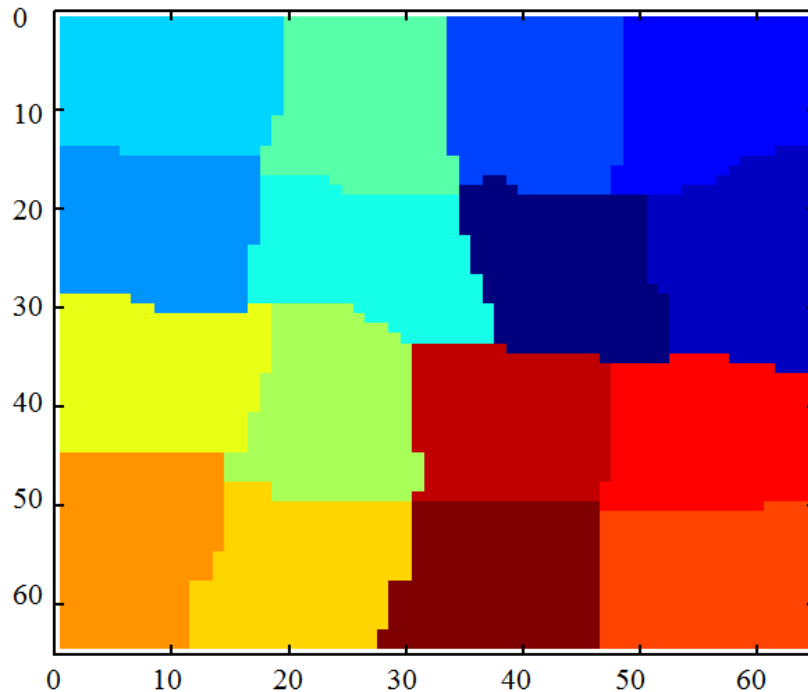
For $N \times N$ mesh on $P \times P$ processor grid:

Usual Cartesian partitioning costs $\sim 4NP$ words moved

MeshPart costs $\sim 3NP$ words moved, 25% savings

Experimental Results: Hypergraph vs. Graph Partitioning

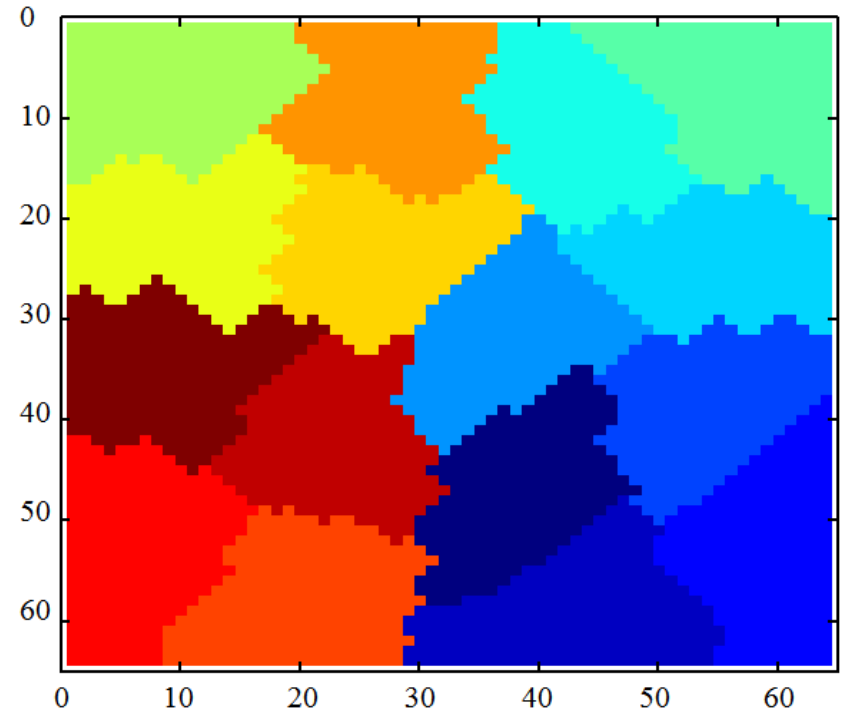
64x64 Mesh (5-pt stencil), 16 processors



Graph Partitioning (Metis)

Total Comm. Vol = 777

Max Vol per Proc = 69



Hypergraph Partitioning (PaToH)

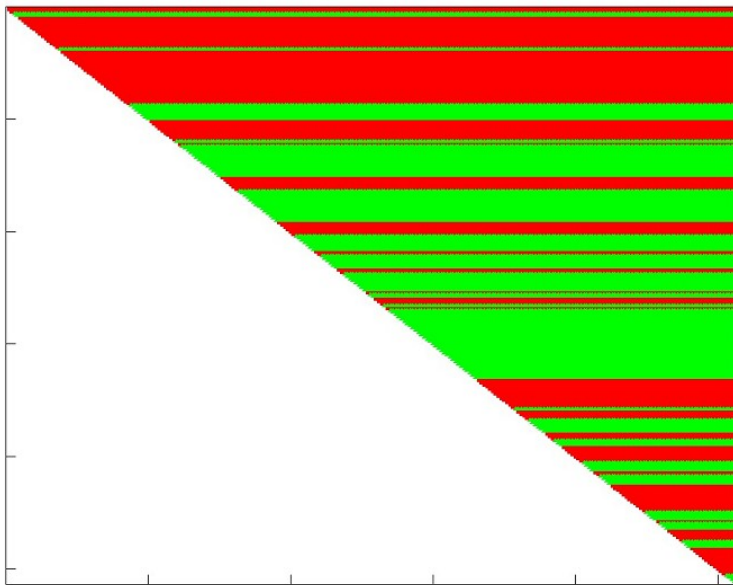
Total Comm. Vol = 719

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

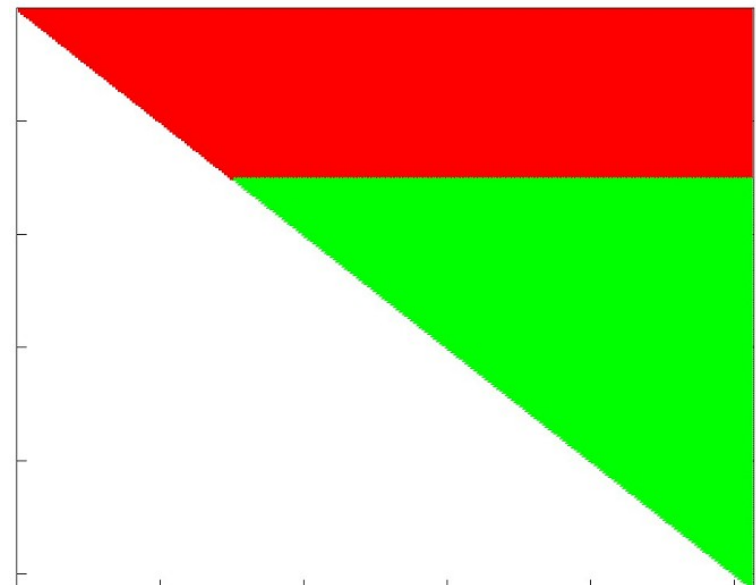
- Graph model of matrix has edge (i,j) if either $A(i,j)$ or $A(j,i)$ nonzero
- Same graph for A as $|A| + |A^T|$
- Ok for symmetric matrices, what about nonsymmetric?
 - Try A upper triangular



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
- For more see Bruce Hendrickson's web page
 - www.cs.sandia.gov/~bahendr/partitioning.html
 - “Load Balancing Fictions, Falsehoods and Fallacies”

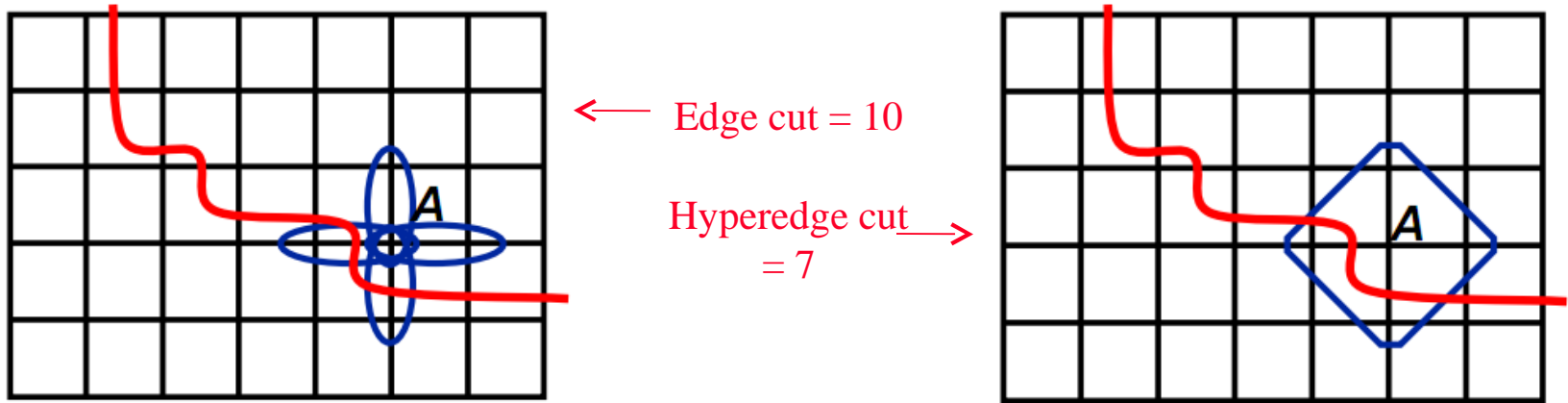
Extra Slides

Beyond Simple Graph Partitioning

- Undirected graphs model symmetric matrices, not unsymmetric ones
- More general graph models include:
 - Hypergraph: nodes are computation, edges are communication, but connected to a set (≥ 2) of nodes
 - HMETIS, PATOH, ZOLTAN packages
 - Bipartite model: use bipartite graph for directed graph
 - Multi-object, Multi-Constraint model: use when single structure may involve multiple computations with differing costs
- For more see Bruce Hendrickson's web page
 - www.cs.sandia.gov/~bahendr/partitioning.html
 - "Load Balancing Myths, Fictions & Legends"

Graph vs. Hypergraph Partitioning

Consider a 2-way partition of a 2D mesh:



The cost of communicating vertex A is 1 – we can send the value in one message to the other processor

According to the graph model, however the vertex A contributes 2 to the total communication volume, since 2 edges are cut.

The hypergraph model accurately represents the cost of communicating A (one hyperedge cut, so communication volume of 1).

Result: Unlike graph partitioning model, the hypergraph partitioning model gives exact communication volume (minimizing cut = minimizing communication)

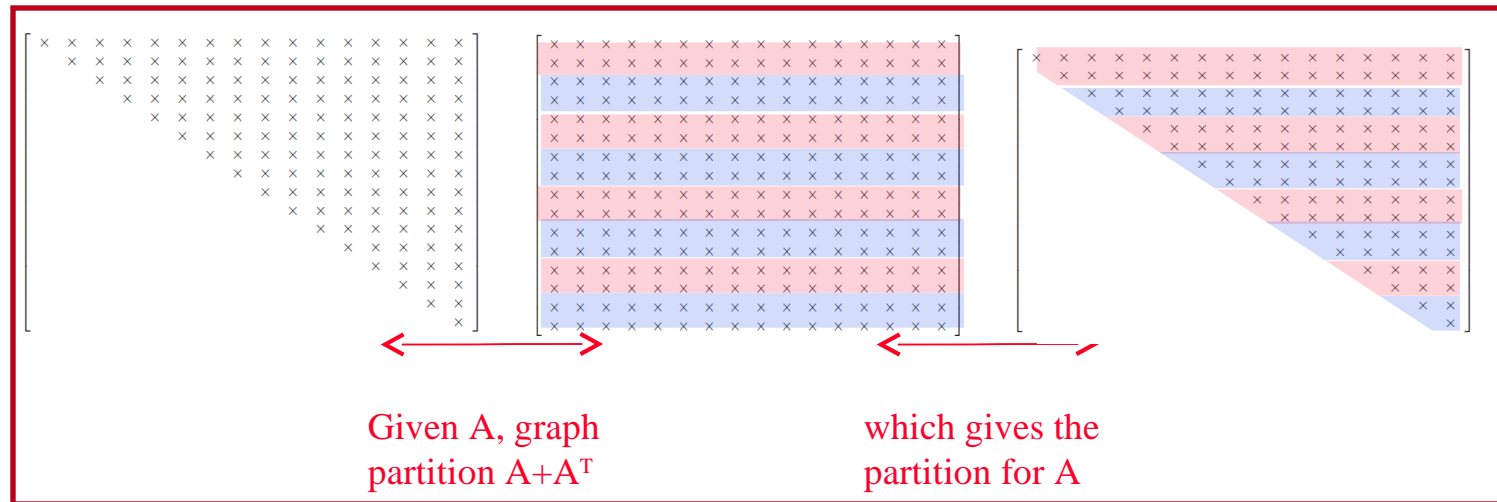
Therefore, we expect that hypergraph partitioning approach can do a better job at minimizing total communication. Let's look at a simple example...

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?

Illustrative Bad Example: triangular matrix

Whereas the hypergraph model can capture nonsymmetry, the graph partitioning model deals with nonsymmetry by partitioning the graph of $A+A^T$ (which in this case is a dense matrix).

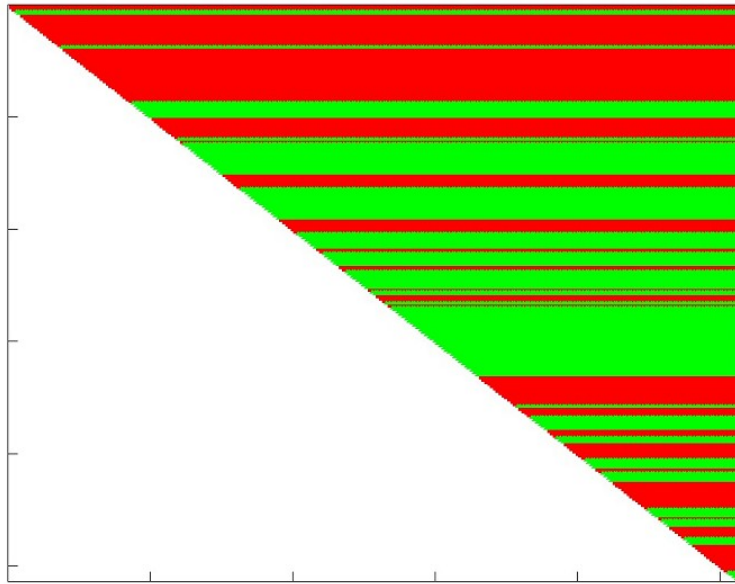


This results in a suboptimal partition in terms of both communication and load balancing. In this case,

Total Communication Volume = 60 (optimal is ~12 in this case, subject to load balancing)

Proc1: 76 nonzeros, Proc 2: 60 nonzeros (~26% imbalance ratio)

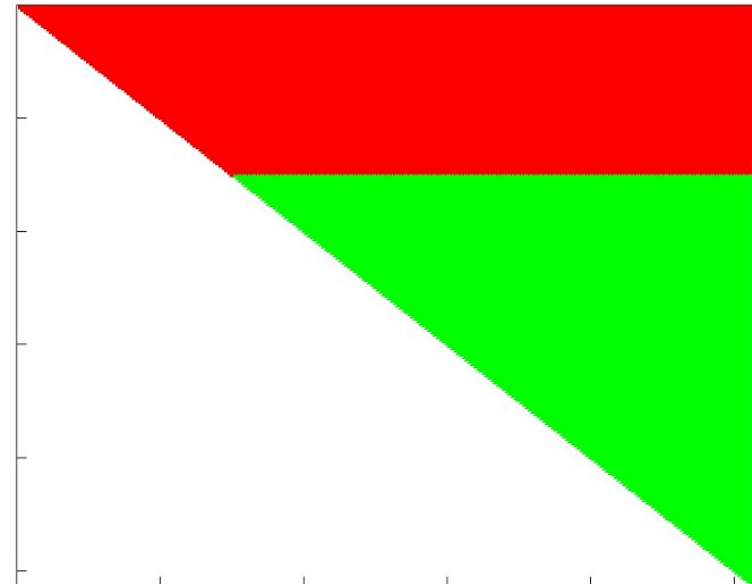
Experimental Results: Illustration of Triangular Example



Graph Partitioning (Metis)

Total Communication Volume= 254

Imbalance ratio = 6%



Hypergraph Partitioning (PaToH)

Total Communication Volume= 181

Imbalance ratio = 0.1%

Conclusions from this section:

- 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

Coordinate-Free Partitioning: Summary

- Several techniques for partitioning without coordinates
 - Breadth-First Search – simple, but not great partition
 - Kernighan-Lin – good corrector given reasonable partition
 - Spectral Method – good partitions, but slow
- Multilevel methods
 - Used to speed up problems that are too large/slow
 - Coarsen, partition, expand, improve
 - Can be used with K-L and Spectral methods and others
- Speed/quality
 - For load balancing of grids, multi-level K-L probably best
 - For other partitioning problems (vision, clustering, etc.) spectral may be better
 - Good software available

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 1: Edge Cut = Communication Cost

- Myth1: The edge-cut deceit
edge-cut = communication cost
- Not quite true:
 - #vertices on boundary is actual communication volume
 - Do not communicate same node value twice
 - Cost of communication depends on # of messages too (α term)
 - Congestion may also affect communication cost
- Why is this OK for most applications?
 - Mesh-based problems match the model: cost is \sim edge cuts
 - Other problems (data mining, etc.) do not

Myth 2: Simple Graphs are Sufficient

- Graphs often used to encode data dependencies
 - Do X before doing Y
- Graph partitioning determines data partitioning
 - Assumes graph nodes can be evaluated in parallel
 - Communication on edges can also be done in parallel
 - Only dependence is between sweeps over the graph
- More general graph models include:
 - Hypergraph: nodes are computation, edges are communication, but connected to a set (≥ 2) of nodes
 - Bipartite model: use bipartite graph for directed graph
 - Multi-object, Multi-Constraint model: use when single structure may involve multiple computations with differing costs

Myth 3: 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
 - Partition should be incremental
 - Change minimally relative to prior one
 - Must not use too much memory
- Example from Touheed, Selwood, Jimack and Bersins
 - 1 M elements with adaptive refinement on SGI Origin
 - Timing data for different partitioning algorithms:
 - Repartition time from 3.0 to 15.2 secs
 - Migration time : 17.8 to 37.8 secs
 - Solve time: 2.54 to 3.11 secs

References

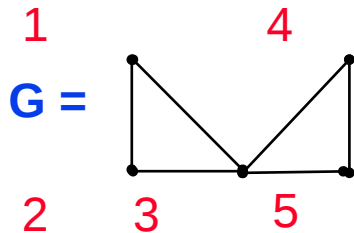
- Details of all proofs on Jim Demmel's 267 web page
- A. Pothen, H. Simon, K.-P. Liou, "Partitioning sparse matrices with eigenvectors of graphs", SIAM J. Mat. Anal. Appl. 11:430-452 (1990)
- M. Fiedler, "Algebraic Connectivity of Graphs", Czech. Math. J., 23:298-305 (1973)
- M. Fiedler, Czech. Math. J., 25:619-637 (1975)
- B. Parlett, "The Symmetric Eigenproblem", Prentice-Hall, 1980
- www.cs.berkeley.edu/~ruhe/lantplht/lantplht.html
- www.netlib.org/laso

Summary

- Partitioning with nodal coordinates:
 - Inertial method
 - Projection onto a sphere
 - Algorithms are efficient
 - Rely on graphs having nodes connected (mostly) to “nearest neighbors” in space
- Partitioning without nodal coordinates:
 - Breadth-First Search – simple, but not great partition
 - Kernighan-Lin – good corrector given reasonable partition
 - Spectral Method – good partitions, but slow
- Today:
 - Spectral methods revisited
 - Multilevel methods

Another Example

- *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
 - $L(G)(i,i) = \text{degree of node } i$ (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



$$L(G) = \begin{pmatrix} 2 & -1 & -1 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ -1 & -1 & 4 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & -1 & 2 \end{pmatrix}$$

Hidden slide

Properties of Incidence and Laplacian matrices

- *Theorem 1:* Given G , $\text{In}(G)$ and $L(G)$ have the following properties
(proof on Demmel's 1996 CS267 web page)
 - $L(G)$ is symmetric. (This means the eigenvalues of $L(G)$ are real and its eigenvectors are real and orthogonal.)
 - Let $\mathbf{e} = [1, \dots, 1]^T$, i.e. the column vector of all ones. Then $L(G) * \mathbf{e} = 0$.
 - $\text{In}(G) * (\text{In}(G))^T = L(G)$. This is independent of the signs chosen for each column of $\text{In}(G)$.
 - Suppose $L(G) * \mathbf{v} = \lambda * \mathbf{v}$, $\mathbf{v} \neq 0$, so that \mathbf{v} is an eigenvector and λ an eigenvalue of $L(G)$. Then

$$\begin{aligned}\lambda &= \|\text{In}(G)^T * \mathbf{v}\|^2 / \|\mathbf{v}\|^2 & \dots \|\mathbf{x}\|^2 = \sum_k x_k^2 \\ &= \sum \{ (\mathbf{v}(i) - \mathbf{v}(j))^2 \text{ for all edges } \mathbf{e} = (i, j) \} / \sum_i \mathbf{v}(i)^2\end{aligned}$$

- 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. In particular, $\lambda_2 \neq 0$ if and only if G is connected.
- *Definition:* $\lambda_2(L(G))$ is the **algebraic connectivity** of G