## CS 267 Applications of Parallel Computers

Lecture 15:
Graph Partitioning - II

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Outline of Graph Partitioning Lectures
${ }^{\circ}$ Review of last lecture
${ }^{\circ}$ Partitioning without Nodal Coordinates - continued

- Kernighan/Lin
- Spectral Partitioning
${ }^{\circ}$ Multilevel Acceleration
- BIG IDEA, will appear often in course
${ }^{\circ}$ Available Software
- good sequential and parallel software availble
${ }^{\circ}$ Comparison of Methods
${ }^{\circ}$ Applications


## Review Definition of Graph Partitioning

${ }^{\circ}$ Given a graph $\mathbf{G}=\left(\mathbf{N}, \mathrm{E}, \mathrm{W}_{\mathrm{N}}, \mathrm{W}_{\mathrm{E}}\right)$

- $N=$ nodes (or vertices), $E=$ edges
- $\mathrm{W}_{\mathrm{N}}=$ node weights, $\mathrm{W}_{\mathrm{E}}=$ edge weights
${ }^{\circ}$ Ex: $\mathrm{N}=\{$ tasks $\}, \mathrm{W}_{\mathrm{N}}=$ \{task costs $\}$, edge ( $\mathrm{j}, \mathrm{k}$ ) in E means task j sends $\mathrm{W}_{\mathrm{E}}(\mathrm{j}, \mathrm{k})$ words to task $k$
${ }^{\circ}$ Choose a partition $N=N_{1} \mathbf{U} \mathbf{N}_{2} \mathbf{U} \ldots \mathbf{U} \mathbf{N}_{\mathrm{P}}$ such that
- The sum of the node weights in each $\mathrm{N}_{\mathrm{j}}$ is "about the same"
- The sum of all edge weights of edges connecting all different pairs $\mathrm{N}_{\mathrm{j}}$ and $\mathrm{N}_{\mathrm{k}}$ is minimized
- Ex: balance the work load, while minimizing communication
- Special case of $\mathbf{N}=\mathbf{N}_{1} \mathbf{U} \mathbf{N}_{2}$ : Graph Bisection



## Review of last lecture

- Partitioning with nodal coordinates
- Rely on graphs having nodes connected (mostly) to "nearest neighbors" in space
- Common when graph arises from physical model
- Algorithm very efficient, does not depend on edges!
- Can be used as good starting guess for subsequent partitioners, which do examine edges
- Can do poorly if graph less connected:
- Partitioning without nodal coordinates
- Depends on edges
- No assumptions about where "nearest neighbors" are
- Began with Breadth First Search (BFS)



## Partitioning without nodal coordinates - Kernighan/Lin

${ }^{\circ}$ Take a initial partition and iteratively improve it

- Kernighan/Lin (1970), cost $=\mathbf{O}\left(|\mathrm{N}|^{3}\right)$ but easy to understand
- Fiduccia/Mattheyses (1982), cost $=\mathbf{O}(|E|)$, much better, but more complicated
${ }^{\circ}$ Let $G=\left(N, E, W_{E}\right)$ be partitioned as $N=A U B$, where $|A|=|B|$
${ }^{\circ} T=\operatorname{cost}(A, B)=\Sigma\{W(e)$ where $e$ connects nodes in $A$ and B\}
${ }^{\circ}$ Find subsets $X$ of $A$ and $Y$ of $B$ with $|X|=|Y|$ so that swapping $X$ and $Y$ decreases cost:
- newA = A - X UY and newB = B - Y UX
- newT = cost(newA , newB) < cost(A,B)
- Keep choosing $X$ and $Y$ until cost no longer decreases
${ }^{\circ}$ Need to compute newT efficiently for many possible $X$ and $Y$, choose smallest


## Kernighan/Lin - Preliminary Definitions

${ }^{\circ} T=\operatorname{cost}(A, B), \quad n e w T=\operatorname{cost}(n e w A$, newB)
${ }^{\circ}$ Need an efficient formula for newT; will use

- $E(a)=$ external cost of $a$ in $A=\Sigma\{W(a, b)$ for $b$ in $B\}$
- $I(a)=$ internal cost of $a$ in $A=\Sigma\left\{W\left(a, a^{\prime}\right)\right.$ for other $a^{\prime}$ in $\left.A\right\}$
- $D(a)=$ cost of $a$ in $A \quad=E(a)-I(a)$
- Moving a from $A$ to $B$ would decrease $T$ by $D(a)$
- $E(b), I(b)$ and $D(b)$ defined analogously for $b$ in $B$
${ }^{\circ}$ Consider swapping $X=\{a\}$ and $Y=\{b\}$
- newA $=A-\{a\} \cup\{b\}$, new $B=B-\{b\} \cup\{a\}$
${ }^{\circ}$ newT $=T-\left(D(a)+D(b)-\right.$ 2* $\left.^{*}(a, b)\right)=T-$ gain(a,b)
- gain(a,b) measures improvement gotten by swapping $a$ and $b$
- Update formulas, after $\mathbf{a}$ and $\mathbf{b}$ are swapped
- newD( $\left.a^{\prime}\right)=D\left(a^{\prime}\right)+2^{*} w\left(a^{\prime}, a\right)-2^{*} w\left(a^{\prime}, b\right)$ for $a^{\prime}$ in $A, a^{\prime}!=a$
- newD( $\left.b^{\prime}\right)=D\left(b^{\prime}\right)+2^{*} w\left(b^{\prime}, b\right)-2^{*} w\left(b^{\prime}, a\right)$ for $b^{\prime}$ in $B, b^{\prime}!=b$


## Kernighan/Lin Algorithm



```
    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|}\mp@subsup{}{2}{~
            Unmark all nodes in N
            ... cost = O(|N|)
            While there are unmarked nodes
                            ... |N//2 iterations
            Find an unmarked pair (a,b) maximizing gain(a,b)
                                ... cost = O(|N|}\mp@subsup{}{}{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
            ... (a1,b1), ..., (ak,bk) and gains gain(1),...., gain(k)
            ... where k = |N|/2, numbered in the order in which we marked them
        Pick m maximizing Gain = \Sigma k=1 to m gain(k)
                            ... cost = O(|N|)
            ...Gain is reduction in cost from swapping (a1,b1) through (am,bm)
        If Gain > 0 then ... it is worth swapping
            Update newA = A - { a1,\ldots,am } U {b1,\ldots,bm } _.. cost = O(|N|)
            Update newB = B - {b1,\ldots,bm } U { a1,...,am } _.. cost = O(|N|)
            Update T = T - Gain
                            ... cost = O(1)
        endif
    Until Gain <= 0

\section*{Comments on Kernighan/Lin Algorithm}
\({ }^{\circ}\) Most expensive line show in red
\({ }^{\circ}\) 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
\({ }^{\circ}\) How many times do we Repeat?
- K/L tested on very small graphs (|N|<=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 \(2^{-\mid N / 30}\)

\section*{Partitioning without nodal coordinates - Spectral Bisection}
- Based on theory of Fiedler (1970s), popularized by Pothen, Simon, Liou (1990)
\({ }^{\circ}\) Motivation, by analogy to a vibrating string
\({ }^{\circ}\) Basic definitions
\({ }^{\circ}\) Vibrating string, revisited
\({ }^{\circ}\) Motivation, by using a continuous approximation to a discrete optimization problem
\({ }^{\circ}\) 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 ...

\section*{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 \(\mathbf{N}\) - and \(\mathrm{N}_{+}\)
- Same idea for other graphs (eg planar graph ~ trampoline)


\section*{Basic Definitions}
- Definition: The incidence matrix \(\ln (\mathrm{G})\) 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 \(\ln (G)\) 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 \(\ln (G)\) by -1 still satisfies the definition, but this won't matter...
\({ }^{\circ}\) 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
- \(L(G)(i, i)=\) degree of node \(I\) (number of incident edges)
- \(L(G)(i, j)=-1\) if \(i!=j\) and there is an edge \((i, j)\)
- \(L(G)(i, j)=0\) otherwise

\section*{Example of \(\ln (\mathrm{G})\) and \(\mathrm{L}(\mathrm{G})\) for 1D and 2D meshes}


Nodes numbered th black
Edges nombered in blue

\section*{Properties of Incidence and Laplacian matrices}
- Theorem 1: Given \(G, \ln (G)\) and \(L(G)\) have the following properties (proof on web page)
- \(L(G)\) is symmetric. (This means the eigenvalues of \(L(G)\) are real and its eigenvectors are real and orthogonal.)
- Let \(\mathrm{e}=[1, \ldots, 1]^{\top}\), i.e. the column vector of all ones. Then \(L(G)^{*} e=0\).
- \(\ln (G){ }^{*}(\ln (G))^{\top}=L(G)\). This is independent of the signs chosen for each column of \(\ln (G)\).
- Suppose \(L(G)^{*} v=\lambda^{*} v\), \(v!=0\), so that \(v\) is an eigenvector and \(\lambda\) an eigenvalue of \(L(G)\). Then
\[
\begin{aligned}
\lambda & =\left\|\ln (\mathrm{G})^{\mathrm{T} *} \mathrm{v}\right\|^{2} /\|\mathrm{v}\|^{2} \\
& =\Sigma\left\{(\mathrm{v}(\mathrm{i})-\mathrm{v}(\mathrm{j}))^{2} \text { for all edges } \mathrm{e}=(\mathrm{i}, \mathrm{j})\right\} / \Sigma_{\mathrm{i}} \mathrm{v}(\mathrm{i})^{2} \quad \cdots\|\mathrm{x}\|^{2}=\Sigma_{\mathrm{k}} \mathrm{x}_{\mathrm{k}}{ }^{2}
\end{aligned}
\]
- The eigenvalues of \(L(G)\) are nonnegative:
\[
-\quad 0=\lambda_{1}<=\lambda_{2}<=\ldots<=\lambda_{n}
\]
- The number of connected components of \(G\) is equal to the number of \(\lambda_{i}\) equal to 0 . In particular, \(\lambda_{2}!=0\) if and only if \(G\) is connected.
\({ }^{\circ}\) Definition: \(\lambda_{2}(\mathrm{~L}(\mathrm{G}))\) is the algebraic connectivity of G

\section*{Spectral Bisection Algorithm}
\({ }^{\circ}\) Spectral Bisection Algorithm:
- Compute eigenvector \(\mathrm{v}_{2}\) corresponding to \(\lambda_{2}(\mathrm{~L}(\mathrm{G}))\)
- For each node \(\mathbf{n}\) of \(\mathbf{G}\)
- if \(\mathbf{v}_{\mathbf{2}}(\mathbf{n})<\mathbf{0}\) put node \(\mathbf{n}\) in partition \(\mathbf{N}\) -
- else put node \(\mathbf{n}\) in partition \(\mathbf{N}_{+}\)
- Why does this make sense? First reasons...
- Theorem 2 (Fiedler, 1975): Let G be connected, and N - and \(\mathrm{N}+\) defined as above. Then N - is connected. If no \(\mathrm{v}_{2}(\mathrm{n})=0\), then \(\mathrm{N}_{+}\)is also connected. (proof on web page)
\({ }^{\circ}\) Recall \(\lambda_{2}(\mathrm{~L}(\mathrm{G}))\) is the algebraic connectivity of \(G\)
- Theorem 3 (Fiedler): Let \(\mathrm{G}_{1}\left(\mathrm{~N}, \mathrm{E}_{1}\right)\) be a subgraph of \(\mathrm{G}(\mathrm{N}, \mathrm{E})\), so that \(\mathrm{G}_{1}\) is "less connected" than G . Then \(\lambda_{2}(L(G))<=\lambda_{2}(L(G))\), i.e. the algebraic connectivity of \(G_{1}\) is less than or equal to the algebraic connectivity of \(G\). (proof on web page)

\section*{Motivation for Spectral Bisection: Vibrating String}
- Vibrating string has modes of vibration, or harmonics
- Modes computable as follows
- Model string as masses connected by springs (a 1D mesh)
- Write down \(F=m a\) 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 \(\mathbf{N}\) - and \(\mathbf{N}_{+}\)
- Same idea for other graphs (eg planar graph ~ trampoline)


\section*{Details for vibrating string}
\({ }^{\circ}\) Force on mass \(j=k^{\star}[x(j-1)-x(j)]+k^{\star}[x(j+1)-x(j)]\)
\[
\begin{equation*}
=-k^{\star}\left[-x(j-1)+2^{*} x(j)-x(j+1)\right] \tag{*}
\end{equation*}
\]
\({ }^{\circ}\) F=ma yields \(m^{*} x^{\prime \prime}(j)=-k^{*}\left[-x(j-1)+2^{*} x(j)-x(j+1)\right]\)
\({ }^{\circ}\) Writing (*) for \(\mathbf{j}=1,2, \ldots, n\) yields
\[
\begin{aligned}
m^{*} \frac{d^{2}}{d x^{2}}\left(\begin{array}{l}
x(1) \\
x(2) \\
\cdots \\
x(j) \\
\cdots \\
x(n)
\end{array}\right)=-k^{*}\left(\begin{array}{l}
2^{*} x(1)-x(2) \\
-x(1)+2^{*} x(2)-x(3) \\
\cdots \\
-x(j-1)+2^{*} x(j)-x(j+1) \\
\ldots \\
2^{*} x(n-1)-x(n)
\end{array}\right)=-k^{*}\left(\begin{array}{ccccc}
2 & -1 & & & \\
-1 & 2 & -1 & & \\
& \cdots & & \\
& & -1 & 2 & -1 \\
& & & \ldots & \\
& & & -1 & 2
\end{array}\right) *\left(\begin{array}{l}
x(1) \\
x(2) \\
\ldots \\
x(j) \\
\cdots \\
x(n)
\end{array}\right)=-k^{*} L^{*}\left(\begin{array}{l}
x(1) \\
x(2) \\
\ldots \\
x(j) \\
\ldots \\
x(n)
\end{array}\right) \\
(-m / k) x^{\prime \prime}=L^{*} x
\end{aligned}
\]

Vibrating Mass Spring System


\section*{Details for vibrating string - continued}
\({ }^{\circ}-(m / k) x^{\prime \prime}=L^{*} x\), where \(x=\left[x_{1}, x_{2}, \ldots, x_{n}\right]^{\top}\)
\({ }^{\circ}\) Seek solution of form \(x(t)=\sin \left(\alpha^{*} t\right){ }^{*} x 0\)
- \(L^{*} \times 0=(m / k)^{*} \alpha^{2}{ }^{*} x 0=\lambda^{*} \times 0\)
- For each integer i , get \(\lambda=2^{*}\left(1-\cos \left(i^{*} \pi /(\mathrm{n}+1)\right), \mathbf{x 0}=\left(\begin{array}{c}\sin \left(1^{*} \mathrm{i}^{*} \pi /(\mathrm{n}+1)\right) \\ \sin \left(2^{*} i^{*} \pi /(\mathrm{n}+1)\right) \\ \ldots \\ \sin ^{*}\left(\mathrm{n}^{*} i^{*} \pi /(\mathrm{n}+1)\right)\end{array}\right)\right.\)
- Thus \(x 0\) is a sine curve with frequency proportional to \(i\)
- Thus \(\alpha^{2}=2^{*} k / m{ }^{*}\left(1-\cos \left(i^{*} \pi /(n+1)\right)\right.\) or \(\alpha \sim \operatorname{sqrt}(k / m)^{*} \pi^{*} i /(n+1)\)
\({ }^{\circ} L=\left(\begin{array}{ccc}2 & -1 & \\ -1 & 2 & -1\end{array} \quad \begin{array}{c}\text { not quite } L(1 D \text { mesh }), \\ \text { but we can fix that } . . .\end{array}\right.\)

\section*{A "vibrating string" for L(1D mesh)}
\({ }^{\circ}\) First equation changes to \(m^{*} x^{\prime \prime}(1)=-k *[-x(2)+2 / x(1)]\)
- First row of Thanges from [ 2-10 ...] to [1-10 ...]
\({ }^{\circ}\) Last equation changes to \(m^{*} x^{\prime \prime}(n)=-k^{*}[-x(n-1)+\lambda x(n)]\)
- Last row of T changes from [ ...0-1 2 ] to [ ... 0-11]
\({ }^{\circ}\) Component \(j\) of \(i\)-th eigenvector changes to \(\cos \left((\mathrm{j}-.5)^{\star}(\mathrm{i}-1)^{\star} \pi / \mathrm{n}\right)\)
"Vibrating String" for Spectral Bisection


\section*{Eigenvectors of L(1D mesh)}

Eigenvector 1 (all ones)


Eigenvector 2


Eigenvector 3




Motivation for Spectral Bisection:
Continuous Approximation to a discrete optimization problem
\({ }^{\circ}\) Use \(L(G)\) to count the number of edges from \(\mathbf{N}\) - to \(\mathbf{N}_{+}\)
\({ }^{\circ}\) Lemma 1: Let \(\mathrm{N}=\mathrm{N}-\mathrm{U} \mathrm{N}_{+}\)be a partition of \(\mathrm{G}(\mathrm{N}, \mathrm{E})\). Let \(x(j)=-1\) if \(j\) is in \(N\) - and \(x(j)=+1\) if \(j\) is in \(N+\). Then (proof on web page)
The number of edges connecting N - and \(\mathrm{N}_{+}\)
\[
\begin{aligned}
& =.25^{*} \mathbf{x}^{\top} * L(G) * x \\
& =.25 * \Sigma_{i, k} \mathbf{x}(\mathrm{i}) * L(G)(\mathrm{i}, \mathrm{k}) * x(\mathrm{k}) \\
& =.25 * \Sigma\left\{(\mathrm{x}(\mathrm{i})-\mathrm{x}(\mathrm{k}))^{2} \text { for all edges }(\mathrm{i}, \mathrm{j})\right\}
\end{aligned}
\]
\({ }^{\circ}\) Restate partitioning problem as finding vector x with entries +1 or -1 such that
- \(\Sigma_{k} \mathbf{x}(\mathrm{k})=0\), i.e. \(\left|\mathrm{N}_{+}\right|=|\mathrm{N}-|\)
- \# edges connecting \(\mathrm{N}+\) to \(\mathrm{N}-=.25^{*} x^{\top *} \mathrm{~L}(\mathrm{G})^{*} x\) is minimized
- Put node j in \(\mathrm{N}+(\) or \(\mathrm{N}-\) ) if \(\mathrm{x}(\mathrm{j})>=0(\) or \(<0)\)

\section*{Converting a discrete to a continuous problem}
\({ }^{\circ}\) Discrete: Find \(x\) with entries +1 or -1 such that
- \(\Sigma_{k} \mathbf{x}(k)=0\), i.e. \(|\mathbf{N}+|=|N-|\)
- \# edges connecting \(\mathrm{N}+\) to \(\mathrm{N}-=.25^{*} \mathrm{x}^{\top *} \mathrm{~L}(\mathrm{G})^{*} \mathrm{x}\) is minimized
- Put node j in \(\mathrm{N}+(\) or N -) if \(\mathrm{x}(\mathrm{j})>=0\) (or \(<0\) )
\({ }^{\circ}\) Continuous: Find x with real entries such that
- \(\Sigma_{k} \mathrm{x}(\mathrm{k})=0\) and \(\Sigma_{\mathrm{k}}(\mathrm{x}(\mathrm{k}))^{2}=|\mathrm{N}| \quad\) (set includes discrete one above)
-. \(25^{*} \mathrm{x}^{\top \star} \mathrm{L}(\mathrm{G})^{*} \mathrm{x}\) is minimized
- Put node j in \(\mathrm{N}_{+}\)(or N -) if \(\mathrm{x}(\mathrm{j})>=0(\) or \(<0)\)
- Theorem 4 (Courant/Fischer "minimax theorem"): \(\mathbf{x}\) satisfying continuous problem is eigenvector \(\mathbf{v}_{2}\), for \(\lambda_{2}\). (proof on web page)
- Theorem 5: The minimum number of edges connecting \(\mathrm{N}_{+}\)and N - in any partitioning with \(\left|\mathbf{N}+\left|=|\mathbf{N}-| \text { is at least } .2^{\star}\right| \mathbf{N}\right|^{*} \lambda_{2}\). (proof on web page)
- The larger the algebraic connectivity \(\lambda_{2}\), the more edges we need to cut to bisect the graph

\section*{Computing \(\mathrm{v}_{2}\) and \(\lambda_{2}\) of \(\mathrm{L}(\mathrm{G})\) using Lanczos}
\({ }^{\circ}\) 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, \(\mathrm{k} \ll \mathbf{n}\)

Choose an arbitrary starting vector \(r\)
\(b(0)=\|r\|\)
\(\mathrm{j}=0\)
repeat
\(\mathrm{j}=\mathrm{j}+1\)
\(q(j)=r / b(j-1) \quad\)... scale a vector
\(\mathbf{r}=\mathbf{A}^{\star} \mathbf{q}(\mathbf{j}) \quad . .\). matrix vector multiplication, the most expensive step
\(r=r-b(j-1)^{*} v(j-1) \quad \ldots\) "saxpy", or scalar*vector + vector
\(a(j)=v(j)^{\top} * r\)
\(r=r-a(j)^{\star} v(j)\)
... dot product
\(\mathrm{b}(\mathrm{j})=\|\mathbf{r}\|\)
... "saxpy"
.... compute vector norm
until convergence ... details omitted
\(T=\left(\begin{array}{llllll}a(1) & b(1) & & & \\ b(1) & a(2) & b(2) & & \\ b(2) & a(3) & b(3) & \\ & \cdots & \cdots & \cdots & \\ & & b(k-2) & \begin{array}{l}a(k-1) \\ b(k-1)\end{array} \\ & & & b(k-1) & a(k)\end{array}\right)\)

\section*{- Approximate A's eigenvalues/vectors using T's}

\section*{References}
\({ }^{\circ}\) Details of all proofs on web page
\({ }^{\circ}\) A. Pothen, H. Simon, K.-P. Liou, "Partitioning sparse matrices with eigenvectors of graphs", SIAM J. Mat. Anal. Appl. 11:430-452 (1990)
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