CS267: Notes for Lecture 23, April 9, 1999

Graph Partitioning, Part 2

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Partitioning Graphs without Coordinate Information (continued)

Spectral partitioning

This is a powerful but expensive technique, based on techniques introduced by Fiedler in the 1970s, but popularized in 1990 by A. Pothen, H. Simon, and K.-P. Liou, "Partitioning sparse matrices with eigenvectors of graphs", SIAM J. Matrix Anal. Appl., 11:430--452.

We will first describe the algorithm, and then give three related justifications for its efficacy. Let G=(N,E) be an undirected, unweighted graph without self edges (i,i) or multiple edges from one node to another. We define two matrices related to this graph.

Definition The *incidence matrix* In(G) of G is an |N|-by-|E| matrix, with one row for each node and one column for each edge. Suppose edge e=(i,j). Then column e of In(G) is zero except for the the i-th and j-th entries, which are +1 and -1, respectively.

Note that there is some ambiguity in this definition, since G is undirected; writing edge e=(i,j) instead of (j,i) is equivalent to multiplying column e of In(G) by -1. We will see that this ambiguity will not be important to us.

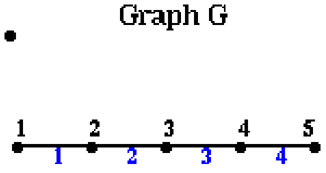
Definition The *Laplacian matrix* L(G) of G is an |N|-by-|N| symmetric matrix, with one row and column for each node. It is defined as follows.

```
  (L(G))(i,j) = degree of node i if i=j
                (number of incident edges)
              = -1   if i!=j and there is an edge (i,j)
              =  0   otherwise
```

Here are some small examples. Note the similarity between the Laplacian graph of the mesh, and the matrix for the discrete Poisson equation, introduced in Lecture 13. With a zero right hand side, we also called this discrete equation Laplace's equation. We will pursue this physical analogy below.

Incidence and Laplacian Matrices

Graph G

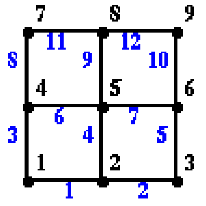


Incidence Matrix In(G)

$$\begin{array}{c|cccc} & 1 & 2 & 3 & 4 \\ \hline 1 & -1 & & & \\ 2 & 1 & -1 & & \\ 3 & & 1 & -1 & \\ 4 & & & 1 & -1 \\ 5 & & & & 1 \end{array}$$

Laplacian Matrix L(G)

$$\begin{array}{c|ccccc} & 1 & 2 & 3 & 4 & 5 \\ \hline 1 & 1 & -1 & & & \\ 2 & -1 & 2 & -1 & & \\ 3 & & -1 & 2 & -1 & \\ 4 & & & -1 & 2 & -1 \\ 5 & & & & -1 & 1 \end{array}$$



$$\begin{array}{c|cccccccccccc} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 & 11 & 12 \\ \hline 1 & -1 & & 1 & & & & & & & & & \\ 2 & 1 & -1 & & 1 & & & & & & & & \\ 3 & & 1 & & & 1 & & & & & & & \\ 4 & & & -1 & & & -1 & & 1 & & & & \\ 5 & & & & -1 & & 1 & -1 & & 1 & & & \\ 6 & & & & & -1 & & 1 & & & 1 & & \\ 7 & & & & & & & & -1 & & & -1 & \\ 8 & & & & & & & & & -1 & & 1 & -1 \\ 9 & & & & & & & & & & -1 & & 1 \end{array}$$

$$\begin{array}{c|ccccccccc} & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\ \hline 1 & 2 & -1 & & -1 & & & & & \\ 2 & -1 & 3 & -1 & & -1 & & & & \\ 3 & & -1 & 2 & & & -1 & & & \\ 4 & -1 & & & 3 & -1 & & -1 & & \\ 5 & & -1 & & -1 & 4 & -1 & & -1 & \\ 6 & & & -1 & & -1 & 3 & & & -1 \\ 7 & & & & -1 & & & 2 & -1 & \\ 8 & & & & & -1 & & -1 & 3 & -1 \\ 9 & & & & & & -1 & & -1 & 2 \end{array}$$

Nodes numbered in black

Edges numbered in blue

The following theorem state some important facts about In(G) and L(G). It introduces us to the idea that the eigenvalues and eigenvectors of L(G) are related to the connectivity of G.

Theorem 1. Given a graph G, its associated matrices In(G) and L(G) have the following properties.

1. L(G) is a symmetric matrix. This means the eigenvalues of L(G) are real, and its eigenvectors are real and orthogonal.
2. Let e=[1,...,1]', where ' means transpose, i.e. the column vector of all ones. Then L(G)*e = 0.
3. In(G)*(In(G))' = L(G). This is independent of the signs chosen in each column of In(G).
4. Suppose L(G)*v = lambda*v, where v is nonzero. Then

$$\texttt{lambda} = \frac{\texttt{norm(In(G)'*v)}^2}{\texttt{norm(v)}^2}$$

$$\texttt{where norm(z)}^2 = \texttt{sum}_\texttt{i}\ \texttt{z(i)}^2$$

$$= \frac{\texttt{sum}_{\texttt{\{all edges e=(i,j)\}}}\ \texttt{(v(i)-v(j))}^2}{\texttt{sum}_\texttt{i}\ \texttt{v(i)}^2}$$

5. The eigenvalues of L(G) are nonnegative: 0 <= lambda_1 <= lambda_2 <= ... <= lambda_n
6. The number of 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.

For a proof of this theorem, click here.

Part 6 of Theorem 1 motivates the following definition.

Definition (M. Fiedler, "Algebraic Connectivity of Graphs", Czech. Math. J. 23:298--305, 1973). lambda_2(L(G)) is called the *algebraic connectivity* of G.

Now we can state our algorithm for spectral bisection of a graph.

```
Compute the eigenvector $v_2$
     corresponding to $lambda_2$ of 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+
   endif
endfor
```

First we show that this partition is at least reasonable, because it tends to give connected components N- and N+:

Theorem 2. (M. Fiedler, "A property of eigenvectors of nonnegative symmetric matrices and its application to graph theory", Czech. Math. J. 25:619--637, 1975.) Let G be connected, and N- and N+ be defined by the above algorithm. Then N- is connected. If no $v_2(n) = 0$, N+ is also connected.

For a partial proof, click here.

There are a number of reasons $lambda_2$ is called the algebraic connectivity. Here is another.

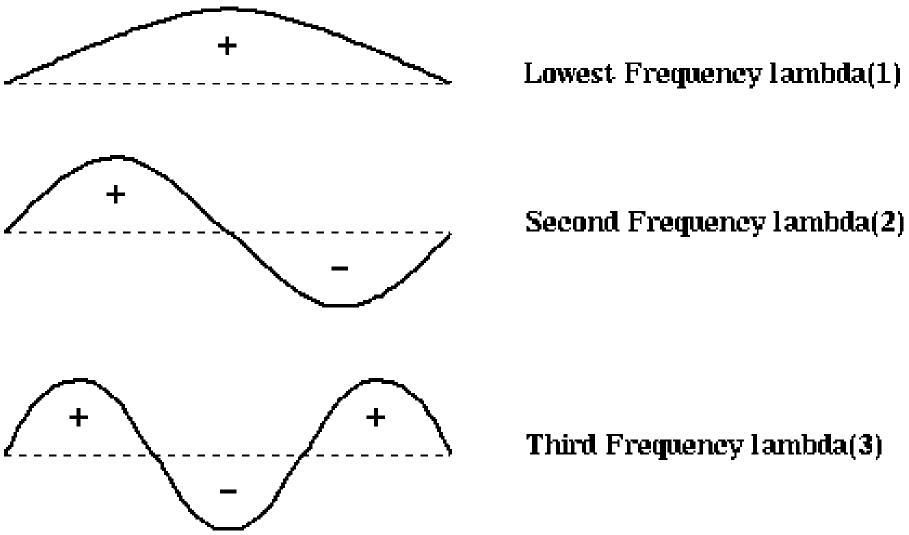
Theorem 3. (Fiedler). Let G=(N,E) be a graph, and $G_1=(N,E_1)$ a subgraph, i.e. with the same nodes and a subset of the edges, so that G_1 is "less connected" than G. Then $lambda_2(L(G_1)) <= lambda_2(L(G))$, i.e. the algebraic connectivity of G_1 is also less than or equal to the algebraic connectivity of G.

We will prove this later, after we introduce more machinery.

Motivation for spectral bisection, by analogy with a vibrating string

How does a taut string vibrate when it is plucked? From our background in either physics or music, we know that it has certain *modes of vibration* or *harmonics*. If we were to take snapshots of these modes, they would look like this:

Modes of a Vibrating String

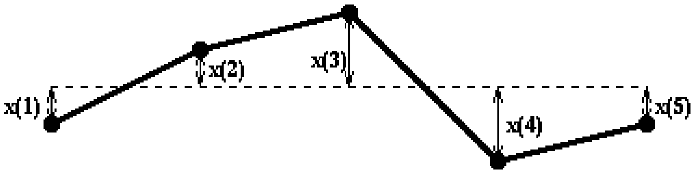

+
Lowest Frequency lambda(1)
+
-
Second Frequency lambda(2)
+
+
-
Third Frequency lambda(3)

Note that we have also labeled each part of the string as to whether it is above the rest position (+), or below (-). In the case of the second frequency $lambda_2$, half the string is labeled +, and half is labeled -, effectively bisecting the string into two equal sized, connected components. It turns out that if we build this vibrating string from a finite set of identical masses (nodes) connected by identical springs (edges), write down Newton's Laws of motion for the masses, and solve for the frequencies and shapes of the vibrational modes, we will get precisely the eigenvalues and eigenvectors of the Laplacian L(G) of the graph G, where G consists of a chain of nodes with nearest neighbor connections. Therefore, the second eigenvector of L(G) is the shape of the second mode of vibration, and divides the graph in half.

In the case of more complicated graphs than simple chains, the same intuition applies. It is easiest to understand in the case of planar graphs, which we can think of as a kind of trampoline; again the second mode of vibration divides the graph (trampoline) into two halves.

Let us perform this construction more explicitly in the case of a string. In the figure below, we let x(i) represent the (small) displacement of mass i from the horizontal.

Vibrating Mass Spring System



If the displacement is small, the force on mass i is

$$\begin{aligned} \text{force}(i) &= k*(x(i-1)-x(i)) + k(x(i+1)-x(i)) \\ &= k*(x(i-1) - 2*x(i) + x(i+1)) \end{aligned}$$

where k is a spring constant. We assume that the spring from x(i) to x(i+1) is stretched proportional to the distance x(i+1)-x(i). If this difference is positive, so mass i+1 is higher than mass i, then the force is upwards, or positive. Newton's law tells us F=ma or

$$\begin{aligned} m * \frac{d^2\, x(i)}{d\, t^2} &= \text{force}(i) \\ &= k*(x(i-1) - 2*x(i) + x(i+1)) \end{aligned}$$

We need to be careful about what happens at the end masses. The simplest, and nearly correct, decision is to fix x(0)=x(n+1)=0 (like a taut spring). This lets us write down the system of ODEs

$$\begin{aligned} \frac{m * d^2}{d\, t^2} \begin{bmatrix} x(1) \\ x(2) \\ .... \\ x(n-1) \\ x(n) \end{bmatrix} &= -k * \begin{bmatrix} 2*x(1)-x(2) \\ -x(1)+2*x(2)-x(3) \\ ... \\ -x(n-2)+2*x(n-1)-x(n) \\ -x(n-1)+2*x(n) \end{bmatrix} \\ &= -k * \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & ... & & & \\ & & -1 & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} * \begin{bmatrix} x(1) \\ x(2) \\ .... \\ x(n-1) \\ x(n) \end{bmatrix} \\ &= -k * M * \begin{bmatrix} x(1) \\ x(2) \\ .... \\ x(n-1) \\ x(n) \end{bmatrix} \end{aligned}$$

or yet more briefly,

$$-(m/k) * \frac{d^2\, x(t)}{d^2\, t} = M * x(t)$$

where x(t) is a vector [x(1),...,x(n)]'. We seek solutions of the form x(t) = sin(a*t)*x0, where a and x0 are a scalar and vector to be determined. Plugging in to the last equation yields

$$(m/k)*a^2*\sin(a*t)*x0 = M * \sin(a*t) * x0$$

Canceling sin(a*t), which is (almost always) zero, yields

$$M * x0 = (m/k)*a^2 * x0 = e * x0$$

Thus x0 is an eigenvector of M and e=(-m/k)*a^2 is an eigenvalue. We know the eigenvalues and eigenvector of M explicitly; as can be confirmed by simple trigonometry, the i-th pair is given by

$$x0 = \begin{bmatrix} \sin(1*i*pi/(n+1)) \\ \sin(2*i*pi/(n+1)) \\ \ldots\ldots \\ \sin((n-1)*i*pi/(n+1)) \\ \sin(n*i*pi/(n+1)) \end{bmatrix}$$

$$e = 2*(1-\cos(i*pi/(n+1)))$$

In other words, we just get sine curves of varying frequencies, exactly matching the curves pictured above. Furthermore, when n is large and i is small,

$$\begin{aligned} (m/k) * a^2 &= e \\ &= 2*(1-\cos(i*pi/(n+1))) \\ &\sim (i*pi/(n+1))^2 \end{aligned}$$

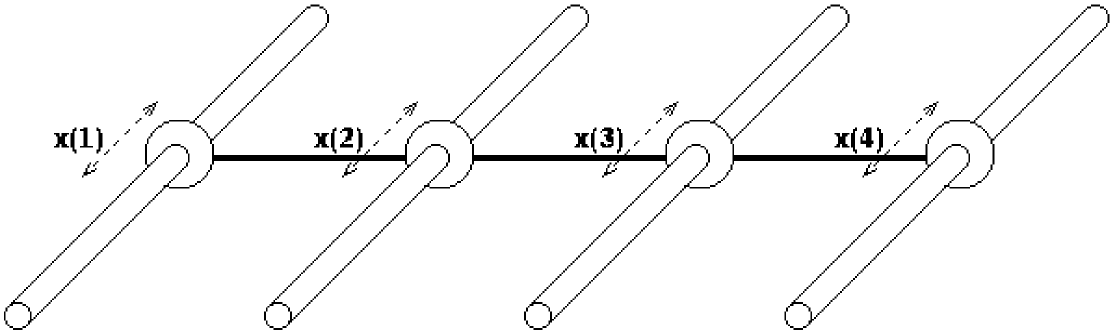
so the frequency of vibration

$$a \sim \mathrm{sqrt}(k/m)*pi/(n+1) * i$$

In other words, the frequencies of successive modes of vibrations are just multiples of the base frequency, thus providing the harmonics we expect from a plucked string.

Unfortunately, M is not quite the Laplacian L(G) of the simple graph G of n nodes connected in a chain; the (1,1) and (n,n) entries are 2 instead of 1. To make the analogy between spectral bisection and the vibrating string exact, we need a slightly different mass-spring system. This is shown in the figure below. There are n horizontal rods, and on each rod a mass m can slide back and forth frictionlessly. These identical masses are connected with identical springs as before. x(i) is the horizontal displacement from rest.

"Vibrating String" for Spectral Bisection



The only difference from before in the equations of motion is for masses 1 and n, the ones at the end. Since they are only tied to one moving mass, rather than one moving mass and one fixed endpoint, we get

$$m * \frac{d^2\ x(1)}{d\ t^2} = \mathrm{force}(1) = k*(x(2) - x(1))$$

and

$$m * \frac{d^2\ x(n)}{} = \mathrm{force}(1) = k*(x(n-1) - x(n))$$

```
          d t^2
```

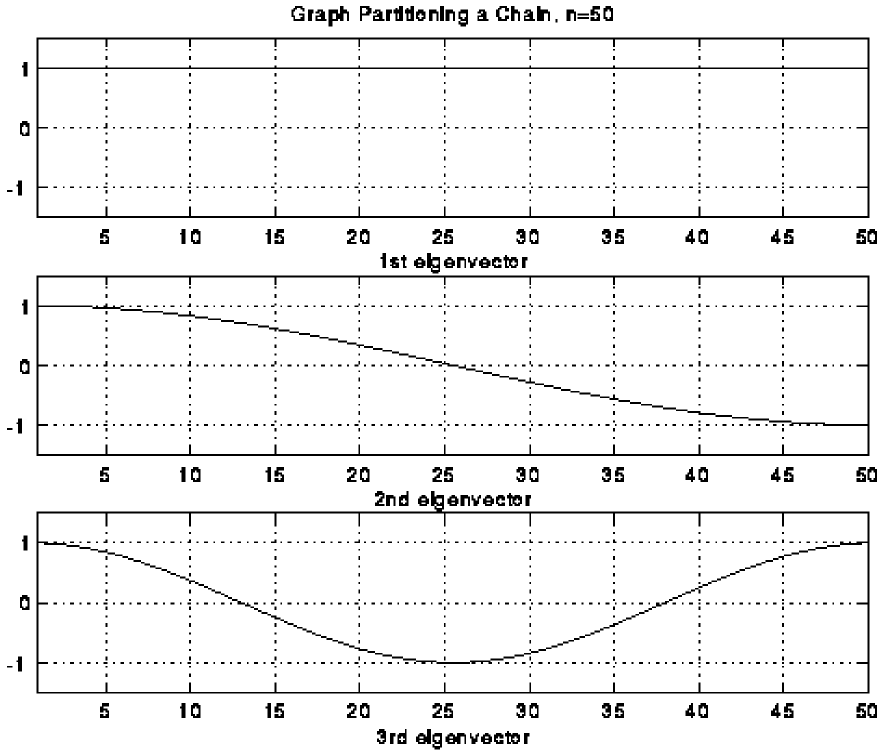
which leads to

```
          [  x(1) ]        [ x(1)-x(2)              ]
  m * d^2 [  x(2) ]        [ -x(1)+2*x(2)-x(3)      ]
  ------  [  .... ] = -k * [       ...              ]
   d t^2  [ x(n-1)]        [ -x(n-2)+2*x(n-1)-x(n)  ]
          [  x(n) ]        [ -x(n-1)+x(n)           ]

                           [  1 -1          ]   [  x(1) ]
                           [ -1 2 -1        ]   [  x(2) ]
                    = -k * [    ...         ] * [ ....  ]
                           [       -1  2 -1 ]   [ x(n-1)]
                           [          -1  1 ]   [  x(n) ]

                                  [  x(1) ]
                                  [  x(2) ]
                    = -k * L(G) * [  .... ]
                                  [ x(n-1)]
                                  [  x(n) ]
```

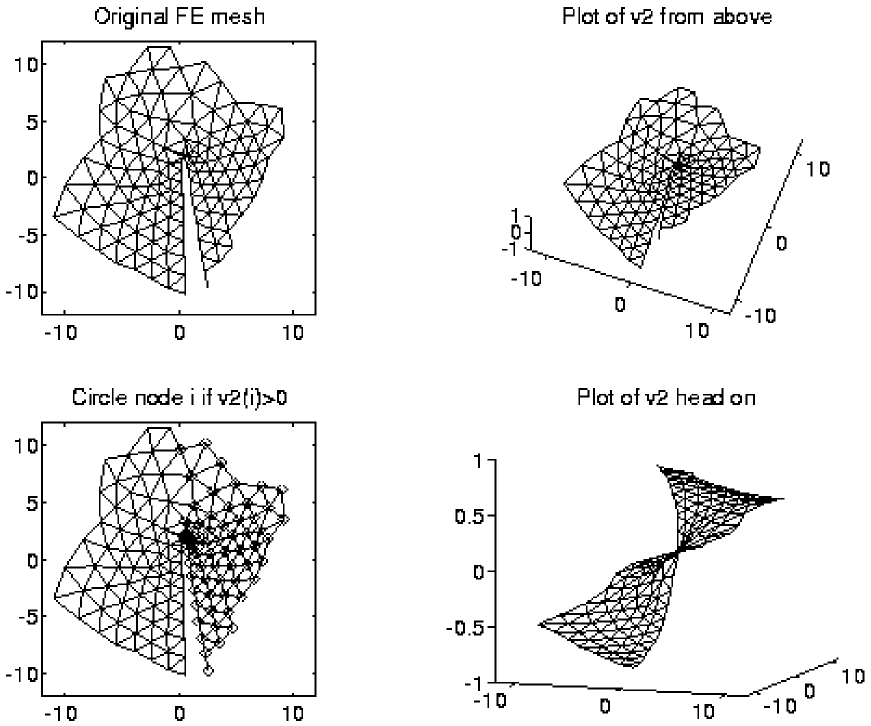
One can again confirm by simple trigonometry, that the i-th eigenvalue and eigenvector of L(G) are given by

```
        [ cos((0+.5) *(i-1)*pi/n) ]
        [ cos((1+.5) *(i-1)*pi/n) ]
   x0 = [ ......                  ]
        [ cos((n-1.5)*(i-1)*pi/n) ]
        [ cos((n-.5) *(i-1)*pi/n) ]

    e = 2*(1-cos((i-1)*pi/n))
```

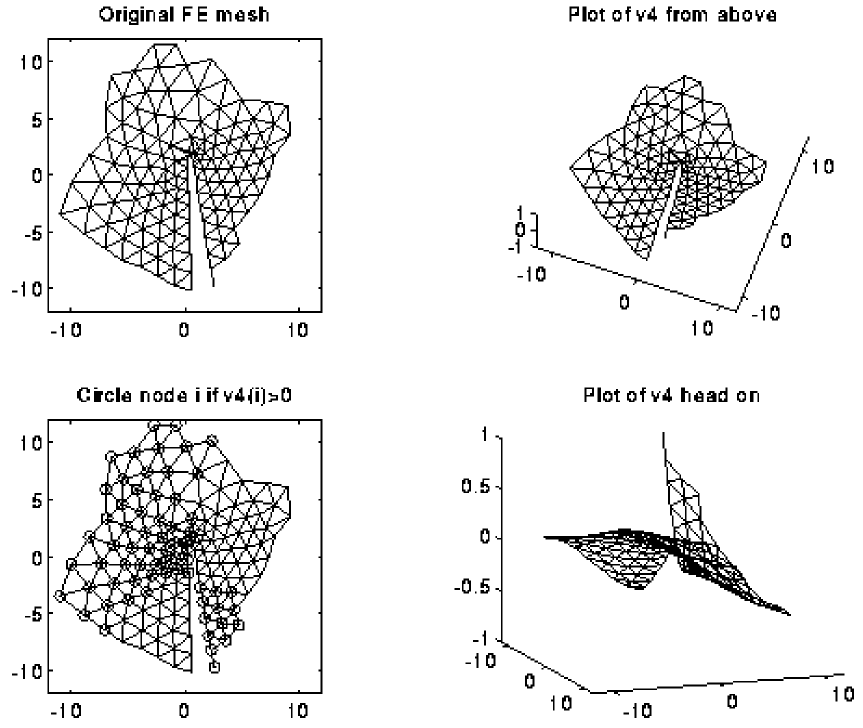
which are just simple cosine curves, the fist few of which are pictured below. Again, the second eigenvector effectively divides the nodes in half.



The same analogy applies to other graphs. For example, here is the same approach applied to a planar graph, which is a simple model of a plate with a crack in it. Physically, one expects the line along the crack to be the weak point, and lead to the second lowest frequency of vibration as the object flexes along the crack, and the second eigenvector picks this out.



From the above pictures, one might also expect higher order eigenvectors to be able to partition a graph into even more parts at a time than 2. This is borne out by examing the 4th eigenvector of the cracked plate, show below. Indeed, many of the results we discuss extend to higher eigenvectors, but we limit our discussion to the second eigenvector, which is most widely used in practice.



Motivation for spectral bisection, by using a real approximation to a discrete optimization problem

We begin with a lemma which shows how to use L(G) to count the number of edges connecting N- and N+ in a partitioned graph G=(N,E), N = N- U N+.

Lemma 1. Let G=(N,E) be a graph, and N = N- U N+ be an arbitrary disjoint partitioning of N. Define a column vector x, with x(i) = +1 if i is in N+, and x(i) = -1 if i is in N-. Let L(G) be the Laplacian of G. Then

```
   # edges connecting N+ and N-
       = .25 * x' * L(G) * x
```

```
        = .25 * sum$_{i,j}$ x(i) * L(G)(i,j) * x(j)
```

This may also be written

```
   # edges connecting N+ and N-
       = .25 * sum$_{\{all edges e=(i,j)\}}$ (x(i) - x(j))$^2$
```

Proof of Lemma 1.

```
  x' * L(G) * x
    = sum$_{i,j}$ L(G)(i,j)*x(i)*x(j)
    = sum$_{i=j}$ L(G)(i,i)*x(i)$^2$  +
      sum$_{i!=j}$ L(G)(i,j)*x(i)*x(j)
    = sum$_{i=j}$ L(G)(i,i)
      +  sum$_{\{i!=j, i, j both in N+ \}}$ L(G)(i,j)*x(i)*x(j)
      +  sum$_{\{i!=j, i, j both in N- \}}$ L(G)(i,j)*x(i)*x(j)
      +  sum$_{\{i!=j, i, j in N- and N+ \}}$ L(G)(i,j)*x(i)*x(j)
    = sum$_i$ degree(i)
      +  sum$_{\{i!=j, i, j both in N+ \}}$ (-1)*(+1)*(+1)
      +  sum$_{\{i!=j, i, j both in N- \}}$ (-1)*(-1)*(-1)
      +  sum$_{\{i!=j, i, j in N- and N+ \}}$ (-1)*(+1)*(-1)
    = 2 * ( #edges in G )
      - 2*( #edges connecting nodes in N+ to nodes in N+ )
      - 2*( #edges connecting nodes in N- to nodes in N- )
      + 2*( #edges connecting nodes in N- to nodes in N+ )
    = 4 * ( #edges connecting nodes in N- to nodes in N+ )
```

To prove the second expression in the lemma, use part 3 of Theorem 1 to note that

```
    x' * L(G) * x = x' * In(G) * (In(G))' * x
                  = sum$_{\{edges e=(i,j)\}}$ ( (In(G))' * x)$_e$ )$^2$
                  = sum$_{\{edges e=(i,j)\}}$ (x(i) - x(j))$^2$
```

This completes the proof. QED

Lemma 1 lets us restate the graph partitioning problem as finding N+ and N-, i.e. a vector x whose entries are +1 or -1, so that

1. | N+ | = | N- |, i.e. sum$_i$ x(i) = 0
2. # edges connecting nodes in N- to nodes in N+ is minimized, i.e. x'*L(G)*x is minimized

or more briefly,

```
   minimum #edges in a partition of N =
        min$_{\{x(i) = +1 or -1, sum_i x(i) = 0\}}$ .25*x'*L(G)*x
```

We will replace this discrete problem by a simpler continuous problem, by minimizing over a larger set of x's than just +-1 vectors, namely all vectors x such that sum$_i$ x(i)^2 = |N|. In other words, we will compute the z minimizing

```
      min$_{\{sum_i z(i)^2 = |N|, sum_i z(i) = 0\}}$ .25*z'*L(G)*z
```

Given z, we will "round it" by computing x(i) = sign(z(i)) to get an assignment.

To see how this is connected to eigenvalues of L(G), we state without proof the following result from linear algebra, which is a special case of the Courant Fischer Minimax Theorem (R. Horn and C. Johnson, "Matrix Analysis", 1988).

Theorem 4. If A is a symmetric matrix with eigenvalues lambda$_1$ <= lambda$_2$ <= ... and eigenvectors v$_1$, v$_2$, ..., then

```
        lambda$_2$ = min$_{\{v != 0,  v'*v_1 = 0\}}$  v'*A*v / v'v
```

and the minimizing v is v$_2$.

For a proof of this special case, click here.

To apply this to graph partitioning, recall that lambda$_1$ = 0 and v$_1$ = [1,...,1]', so the condition v'*v$_1$=0 is the same as sum$_i$ v(i) = 0. Substituting v = z/sqrt(|N|) above yields

```
  min_{sum_i z(i)^2 = |N|, sum_i z(i) = 0} .25*z'*L(G)*z
     = min_{sum_i v(i)^2 = 1, sum_i v(i) = 0} .25*|N|*v'*L(G)*v
                                                 .25*|N|*v'*L(G)*v
     = min_{sum_i v(i)^2 = 1, sum_i v(i) = 0} -----------------
                                                        v'*v
                since v'*v = sum_i v(i)^2 = 1
     = .25 * |N| *
                                             v'*L(G)*v
       min_{sum_i v(i)^2 = 1, v'*v_1 = 0} ---------
                                                v'*v
     = .25 * |N| * lambda_2
```

We have nearly proven

Theorem 5. The minimum # edges connecting N+ and N- in any partitioning of G=(N,E) into equal parts N = N+ U N-, is at least .25 * |N| * lambda$_2$.

So the larger the "algebraic connectivity" lambda$_2$, the more edges we need to cut to separate the graph.

Proof of Theorem 5. The minimum number of edges is

```
      min_{x(i) = +1 or -1, sum_i x(i) = 0} .25*x'*L(G)*x
   >= min_{sum_i x(i)^2 = |N|, sum_i x(i) = 0} .25*x'*L(G)*x
         since we are minimizing over
         a larger set of vectors x
    = .25 * |N| * lambda_2
```

QED

In the case of a chain of n nodes, we stated earlier that lambda$_2$ = 2*(1-cos(pi/n)) ~ (pi/n)^2 so the lower bound in Theorem 5 is about .25 * pi^2 / n, which is low by a factor of n. For an d-dimensional grid with n^d nodes, it turns out lambda$_2$ is exactly d times as large as lambda$_2$ for a chain, and again the lower bound of Theorem 5 is about n times too low (O(n^{d-2}) instead of n^{d-1}). For a star graph (n-1 nodes all connected to a single, n-th node) or a complete graph (all nodes connected to all other nodes), the lower bound is nearly exact.

Now we return to the proof of Theorem 3. It is easy using part 3 of Theorem 1 and Theorem 4. Let G be a graph, and G$_1$ a subgraph with the same nodes but a subset of the edges. Let G$_2$ be another subgraph with the same nodes and the complementary set of edges. Let In(G$_1$) and In(G$_2$) be the incidence matrices of G$_1$ and G$_2$, respectively. It is easy to see that In(G) = [In(G$_1$) , In(G$_2$)], if we number the edges in G$_1$ before the edges in G$_2$. Therefore, by part 3 of Theorem 1,

```
    L(G) = In(G) * (In(G))'
         = [ In(G_1) , In(G_2) ] * [ In(G_1) , In(G_2) ]'
         = In(G_1) * (In(G_1))' + In(G_2) * (In(G_2))'
         = L(G_1) + L(G_2)
```

Thus, by Theorem 4,

```
  lambda_2(G)
    = min_{v != 0, sum_i v(i) = 0} v'*L(G)*v / v'*v
    = min_{v != 0, sum_i v(i) = 0} v'*(L(G_1)+L(G_2))*v / v'*v
   >=   min_{v != 0, sum_i v(i) = 0} v'* L(G_1) *v / v'*v
      + min_{v != 0, sum_i v(i) = 0} v'* L(G_2) *v / v'*v
            since we are minimizing over
            a larger set of vectors
    = lambda_2(G_1) + lambda_2(G_2)
   >= lambda_2(G_1)
```

This completes the proof of Theorem 3.

Computing lambda$_2$ and v$_2$ of L(G) using Lanczos

We need a method for computing v$_2$ of L(G). We do not need a particularly accurate answer, because we are only going to use the sign bit of each component to perform the partitioning. If we treat L(G) as a dense matrix, there are algorithms that run in (4/3)*|N|^3 time (for example, routine eig in Matlab, or dsyevx in LAPACK or pdsyevx in ScaLAPACK). Since we started with a graph with relatively few connections compared to a complete graph (which corresponds to a dense L(G)), this is clearly not cost effective.

The algorithm of choice for this problem is Lanczos. Given any n-by-n sparse symmetric matrix A, Lanczos computes a k-by-k symmetric tridiagonal matrix T, whose eigenvalues are good approximations of the eigenvalues of T, and whose eigenvectors can be used to get approximate eigenvectors of A. Building T requires k matrix-vector multiplications with A; this is typically the most expensive part of the algorithm. One hopes to get a good enough approximation with k much small than n. This means one only approximates a small subset of k of A's n eigenvalues. Fortunately, the ones which converge first are the largest and the smallest, including lambda$_2$.

There are many variations on Lanczos. We present the simplest possible version below, and refer the reader to the literature for details. See, for example, "The Symmetric Eigenvalue Problem", B. Parlett, Prentice Hall, 1980. You may also see on-line help page for Lanczos, which is experimental and is likely to move in the future.

```
Choose an arbitrary starting vector r
b(0) = norm(r) = sqrt( $sum_i r(i)^2$ )
i = 0
repeat
  i = i+1
  v(i) = r / b(i-1)
  r = A * v(i)              ... matrix-vector multiply,
                            ...   the most expensive step
  r = r - b(i-1)*v(i-1)     ... "saxpy", costs 2n flops
  a(i) = v(i)' * r          ... dot-product, costs 2n flops
  r = r - a(i)*v(i)         ... "saxpy", costs 2n flops
  b(i) = norm(r)
until convergence           ... details omitted
```

At each step i, the algorithm computes a tridiagonal matrix

```
      [ a(1) b(1)                         ]
      [ b(1) a(2) b(2)                    ]
  T = [      b(2) a(3) b(3)               ]
      [           ...                     ]
      [           b(i-2) a(i-1) b(i-1)    ]
      [                  b(i-1) a(i)      ]
```

whose eigenvalues approximate the eigenvalues of A. Let w(2) be the second eigenvector of T. Then the corresponding approximate eigenvector of A is

$$\mathrm{sum}_{j=1,...,i}\ w(2)(j) * v(j)$$

The reader may already have noticed an irony of using this algorithm to compute v$_2$. One of the major motivations of graph partitioning was to accelerate matrix-vector multiplication by a symmetric matrix M. We are proposing to form the graph G(M), then its Laplacian L(G(M)), and then multiply by L(G(M)) repeatedly in the Lanczos algorithm. But M and L(G(M)) have the same pattern of nonzero entries, so multiplying by L(G(M)) is as hard as multiplying by M. Therefore, spectral partitioning via Lanczos is of use only when one expects to multiply by M many more times than by L(G(M)).

Accelerating Graph Partitioning Using A Multilevel Approach

As mentioned in Lecture 20, many of the previously discussed methods can be accelerated by using the same idea that made multigrid such a fast algorithm for solving the Poisson equation: we will replace the problem of partitioning the original graph G$_0$ = (N$_0$,E$_0$) by the simpler problem of partitioning a *coarse approximation* G$_1$ = (N$_1$,E$_1$) to G$_0$. Given a partitioning of G_1, we will use that to get a starting guess for a partitioning of G_0, and refine it by an iterative process, like Kernighan-Lin. The problem of partitioning G_1 (or more generally G_i) is solved recursively, by approximating it by a yet coarser graph G_2 (or G_{i+1}).

To summarize, we may use divide-and-conquer to partition $G_0 = (N_0,E_0)$ as follows: G=(N,E) as follows:

```
   ( N+, N- ) = Recursive_partition( N, E )
   ... recursive partitioning routine returns N+ and N-
   ... where N = N+ U N-
       If |N| is small
           Partition G=( N, E ) directly to get N = N+ U N-
           Return ( N+, N- )
       else
(1)        Compute a coarse approximation $G_c$ = ( $N_c$, $E_c$ )
(2)        ( $N_c$+ , $N_c$- ) = Recursive_partition( $N_c$, $E_c$ )
(3)        Expand ( $N_c$+, $N_c$- ) to a partition ( N+, N- )
(4)        Improve the partition ( N+, N- )
           Return ( N+, N- )
       endif
```

Steps (1), (3) and (4) in the above algorithm require further explanation. We describe two approaches to implementing these steps. The first approach is described in ``A fast and high quality multilevel scheme for partitioning irregular graphs'', by G. Karypis and V. Kumar; a software package implementing this method (among others) is called METIS. A similar algorithm is available in Chaco, and described in A multilevel algorithm for partitioning graphs, B. Hendrickson and R. Leland, Proc. Supercomputing '95.

The second approach is described in "A fast multilevel implementation of recursive spectral bisection for partitioning unstructured problems" by Barnard and Simon, Proceedings of the 6th SIAM Conference on Parallel Processing for Scientific Computing, 1993.

Multilevel Kernighan-Lin

G_c is computed in step (1) of Recursive_partition as follows. We define a **matching** of a graph G=(N,E) as a subset E_m of the edges E with the property that no two edges in E_m share an endpoint. A **maximal matching** is one to which no more edges can be added and remain a matching. We can compute a maximal matching by a simple random algorithm:

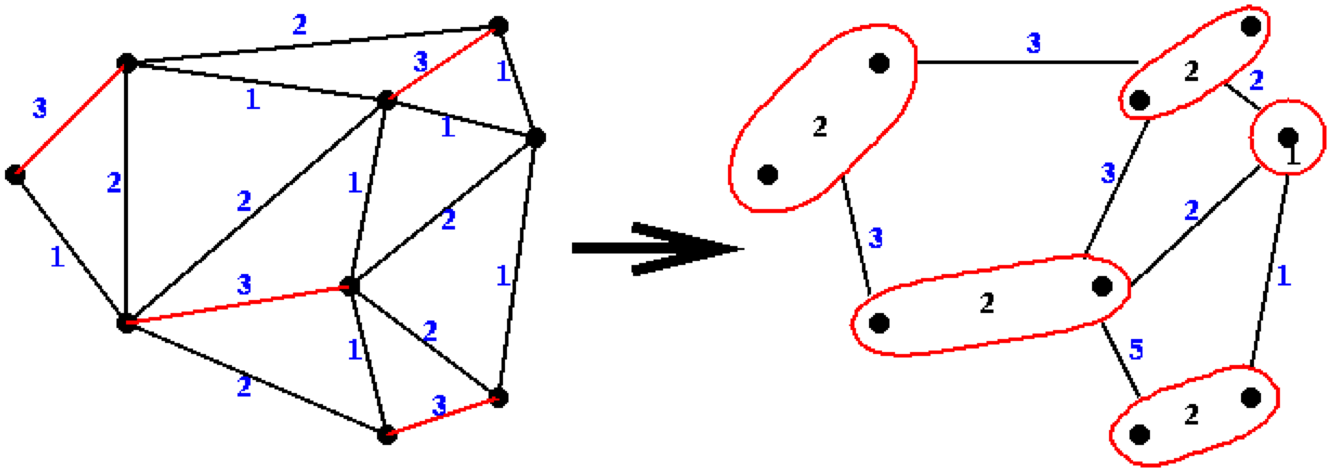
```
   let $E_m$ be empty
   mark all nodes in N as unmatched
   for i = 1 to |N| ... visit the nodes in a random order
     if node i has not been matched,
        choose an edge e=(i,j) where j is also unmatched,
           and add it to $E_m$
        mark i and j as matched
     end if
  end for
```

Given a matching, G_c is computed as follows. We let there be a node r in N_c for each edge in E_m. Then we construct E_c as follows:

```
  for r = 1 to |$E_m$| ... for each node in $N_c$
      let (i,j) be the edge in $E_m$ corresponding to node r
      for each other edge e=(i,k) in E incident on i
         let $e_k$ be the edge in $E_m$ incident on k, and
             let $r_k$ be the corresponding node in $N_c$
         add the edge (r,$r_k$) to $E_c$
      end for
      for each other edge e=(j,k) in E incident on j
         let $e_k$ be the edge in $E_m$ incident on k, and
             let $r_k$ be the corresponding node in $N_c$
         add the edge (r,$r_k$) to $E_c$
      end for
  end for
  if there are multiple edges between pairs of nodes of
       Nc, collapse them into single edges
```

Note that we can take node weights into account by letting the weight of a node (i,j) in N_c be the sum of the weights of the nodes i and j. We can similarly take edge weights into account by letting the weight of an edge in E_c be the sum of the weights of the edges "collapsed" into it. Furthermore, we can choose the edge (i,j) which matches j to i in the construction of N_c above to have the large weight of all edges incident on i; this will tend to minimize the weights of the cut edges. This is called *heavy edge matching* in METIS, and is illustrated below.

How to coarsen a graph using a maximal matching



$G = (N, E)$ | $G_c = (N_c, E_c)$

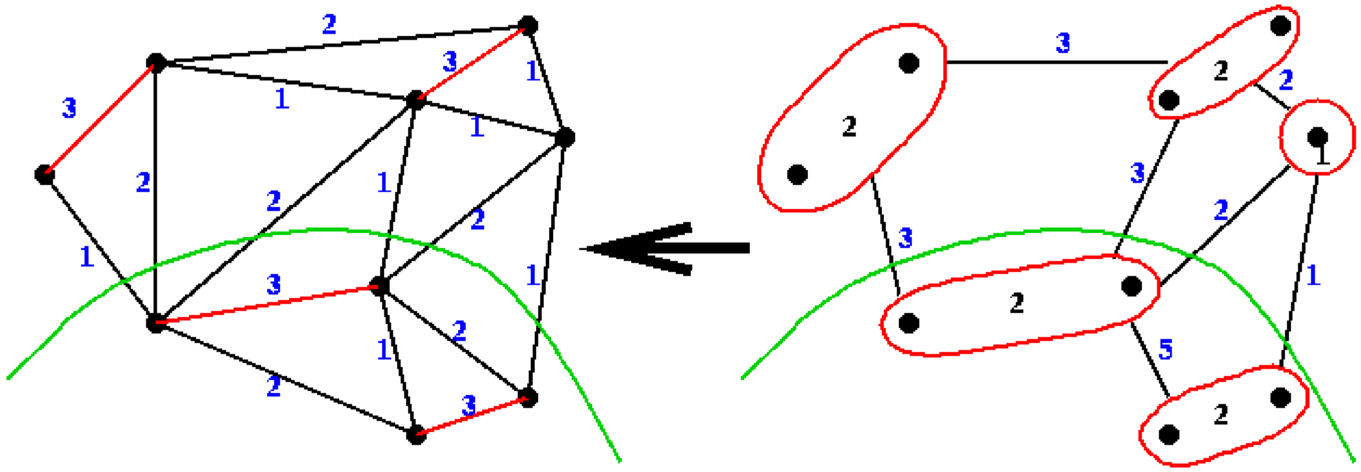
E_s is shown in red | N_s is shown in red

Edge weights shown in blue | Edge weights shown in blue

Node weights are all one | Node weights shown in black

Given a partition (N_c+,N_c-) from step (2) of Recursive_partition, it is easily expanded to a partition (N+,N-) in step (3) by associating with each node in N_c+ or N_c- the nodes of N that comprise it. This is again shown below:

Converting a coarse partition to a fine partition



Partition shown in green

Finally, in step (4) of Recurive_partition, the approximate partition from step (3) is improved using a variation of Kernighan-Lin.

Multilevel Spectral Partitioning

Now we turn to the divide-and-conquer algorithm of Barnard and Simon, which is based on spectral partitioning rather than Kernighan-Lin. The expensive part of spectral bisection is finding the eigenvector v_2, which requires a possibly large number of matrix-vector multiplications with the Laplacian matrix L(G) of the graph G. The divide-and-conquer approach of Recursive_partition will dramatically decrease the cost.

Barnard and Simon perform step (1) of Recursive_partition, computing $G_c = (N_c,E_c)$ from G=(N,E), slightly differently than above: They find a *maximal independent subset N_c of N*. This means that

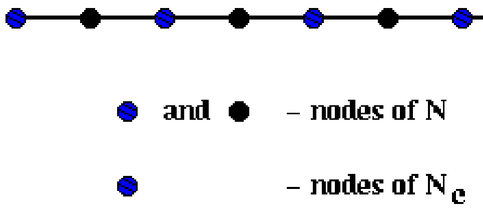
- N contains N_c and E contains E_c,
- no nodes in N_c are directly connected by edges in E (independence), and
- N_c is as large as possible (maximality).

There is a simple "greedy" algorithm for finding an N_c:

```
$N_c$ = empty set
for i = 1 to |N|
   if node i is not adjacent to any node already in $N_c$
      add i to $N_c$
   end if
end for
```

This is shown below in the case where G is simply a chain of 9 nodes with nearest neighbor connections, in which case N_c consists simply of every other node of N.

Maximal Independent Subset N_c of N

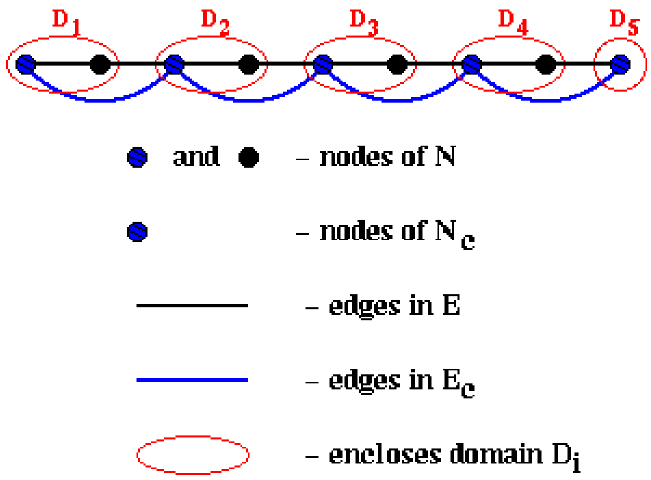


To build E_c, we proceed as follows: We will loop through the edges in E, growing "domains" D_i around each node i in N_c. In other words, a domain consists of the subgraph of G connected to i by the edges examined so far. We will add an edge to E_c whenever an edge in E would connect two of these domains.

```
$E_c$ = empty set
for all nodes i in $N_c$
   $D_i$ = ( { i }, empty set )  ... build initial domains
end for
unmark all edges in E
repeat
   choose an unmarked edge e=(i,j) from E
   if exactly one of i and j (say i) is in some $D_k$
      mark e
      add j and e to $D_k$
   else if i and j are in different $D_k$s (say $D_{k_i}$ and $D_{k_j}$)
      mark e
      add an edge ($k_i$,$k_j$) to $E_c$
   else if both i and j are in the same $D_k$
      mark e
      add it to $D_k$
   else
      leave e unmarked
   endif
until no unmarked edges
```

For example, suppose we start with G being a chain of nodes as above, with nodes and edges numbered from left to right. Then domain D_i for node i will just contain its neighbor to the right, and the edges in E_c will simply connect adjacent nodes in N_c, so G_c is just the chain of length n/2.

Computing G_c from G

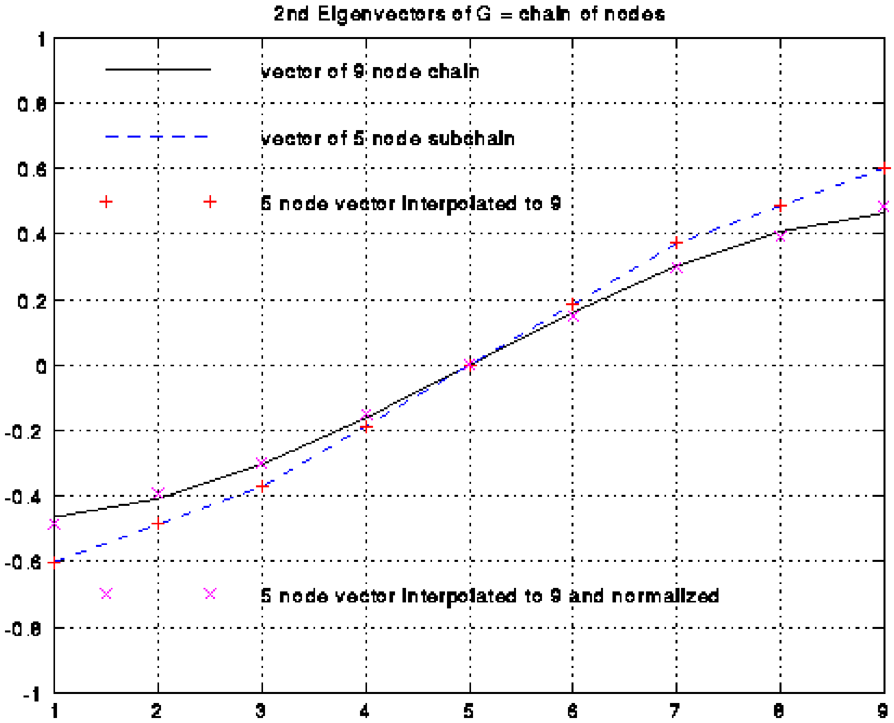


This completes the discussion of Barnard and Simon's implementation of step (1) of Recurive_partition.

Here is how Barnard and Simon implement step (3). Recall that the partitioning is done by using the signs of the components of the second eigenvector of the Laplacian. Assuming that we have computed an approximate second eigenvector v_2 (G_c) of G_c, we must compute an approximate second eigenvector v_2 (G) of G. This is done by interpolation:

```
for each node i in N
   if i is also a node in $N_c$, then
      $v_2$(G)(i) = $v_2$($G_1$)(i),
         ... i.e. use the same eigenvector component
   else
      $v_2$(G)(i) = average of $v_2$($G_1$)(j)
         for all neighbors j of i in $N_c$.
   end if
end for
```

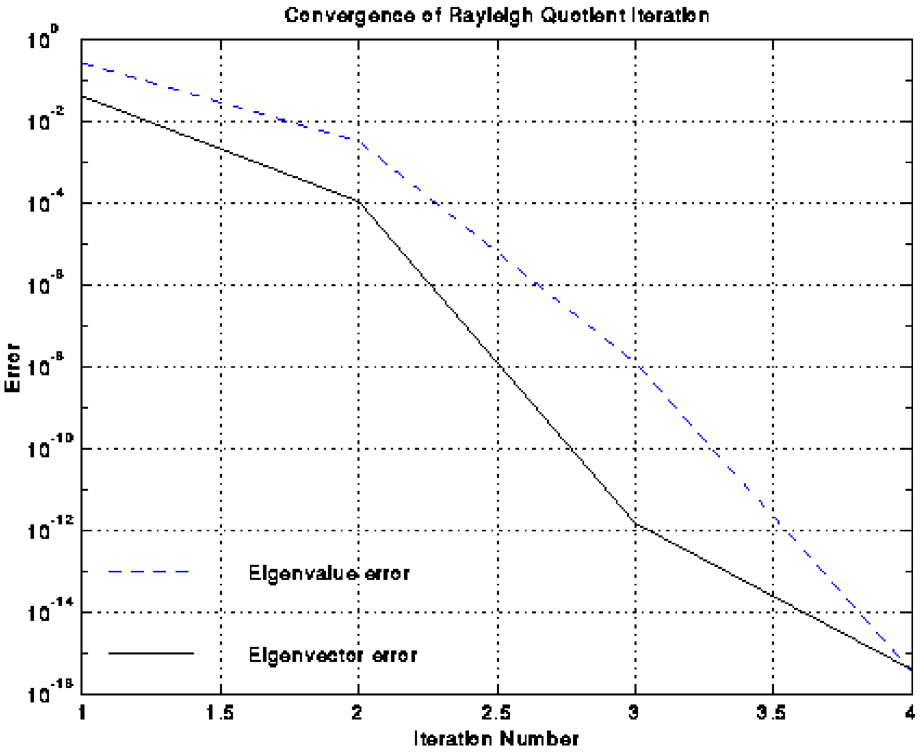
This is shown below in the case of the chain of 9 nodes. The black line is the exact v_2(G) (normalized so the sum-of-squares is one). The dashed blue line is the exact v_2(G_c), also normalized, and which only connects every other node. The red +'s are the approximate v_2(G) computed by interpolation as above, which by construction lie on top of the blue line. The magenta x's are the red +'s normalized, to better see how well they approximate the black line.



Step (4) of Recursive_partition involves refining this approximate second eigenvector to be more accurate. Refining the approximate second eigenvector can be done in several ways. (The unrefined approximate second eigenvector is not always as good as in the case of the chain!). One possibility is that the Lanczos algorithm mentioned above benefits from having a starting vector which mostly points in the direction of the desired eigenvector. More aggressively, one can use a technique called *Rayleight Quotient Iteration*, which uses the fact that the iteration

```
choose a starting vector v(0)
        ... we use $v_2$($G_c$)
v(0) = v(0) / norm2(v(0))
        ... norm2(x) = sqrt($\text{sum}_i$ x(i)$^2$)
i=0
repeat
   i = i+1
   rho(i) = v(i-1)' * L(G) * v(i-1)
        ... rho(i) = Rayleigh Quotient
   v(i) = ( L(G) - rho(i)*I )$^{-1}$ * v(i-1)
   v(i) = v(i) / norm2(v(i))
until convergence
```

converges asymptotically *cubically* to an eigenvalue-eigenvector pair (rho(i),v(i)); this means the the error cubes at every step, so that for example an error of 10^{-4} turns into an error of $(10^{-4})^3 = 10^{-12}$ after one step. rho(i) costs one matrix-vector multiply. Computing v(i), i.e. solving the linear system (L(G) - rho(i)*I) * v(i) = v(i-1), is done using an iterative method (called SYMMLQ) which requires yet more matrix-vector multiplications. But since cubic convergence is so fast, very few steps are needed. This speedy convergence is illustrated below by the example of the chain, where the black line is the error in the approximate eigenvector v(i) and the dashed blue line is the error in the approximate eigenvalue rho(i), as functions of i. One can see the cubic convergence between iterations i=2 and i=3, where the eigenvector error goes from 10^{-4} to 10^{-12}. Cubic convergence is only visible for this one step before hitting the accuracy limit of 10^{-16} due to roundoff.



Experiments report a 10x speedup over the basic spectral bisection algorithm.

Performance Comparison of Different Partitioning Algorithms

Several authors have performed extensive numerical experiments to compare various algorithms based both on

1. the quality of partitions produced (the number of edges cut), and
2. the time taken to compute the partition.

For example, see "Geometric Mesh Partitioning: Implementation and Experiments", by J. Gilbert, G. Miller, and S-H. Teng, and ``A fast and high quality multilevel scheme for partitioning irregular graphs", by G. Karypis and V. Kumar. In addition, a large number of test graphs are available on-line for testing purposes (supplied by Gilbert et al, and Karypis and Kumar).

Recall that there are two classes of algorithms: *geometric algorithms*, that use coordinate information associated with nodes of the graph, and *coordinate-free algorithm*, that do not use this information. Accordingly, we present two studies comparing geometric algorithms, as well as coordinate-free ones.

We begin with geometric algorithms. The following data is taken from "Geometric Mesh Partitioning: Implementation and Experiments". Table 1 below describes the 7 graphs being partitioned. All are meshes in 2 or 3 dimensional space, rather than completely general graphs. The first four are 2-dimensional, and the last two are 3 dimensional. The fifth graph, PWT, is sometimes called "two-and-a-half dimensional", because it is a thin ("almost 2D") surface lying in 3D space. The last two columns give the number of vertices and edges in the graphs. The columns labeled "Grading" says how much larger the longest edges in the graph are than the shortest edges. For example, TRIANGLE is a regular tesselation of the place by identical equilateral triangles, so its grading is 1. AIRFOIL2 is similar to the NASA Airfoil we have seen so often, which has some large and some tiny triangles, the largest 1.3e5 times larger than the smallest.

Mesh	Description	Mesh Type
TAPIR	Cartoon animal	2-D acute triangles
AIRFOIL2	Three-element airfoil	2-D triangles
TRIANGLE	Equilateral triangle	2-D triangles/same size
AIRFOIL3	Four-element airfoil	2-D triangles
PWT	Pressurized wind tunnel	Thin shell in 3-space
BODY	Automobile body	3-D volumes and surfaces
WAVE	Space around airplane	3-D volumes and surfaces

Mesh	Grading	Vertices	Edges
TAPIR	8.5e4	1024	2846
AIRFOIL2	1.3e5	4720	13722
TRIANGLE	1.0e0	5050	14850
AIRFOIL3	3.0e4	15606	45878
PWT	1.3e2	36519	144794
BODY	9.5e2	45087	163734
WAVE	3.9e5	156317	1059331

Table 1: Test problems. "Grading" is the ratio of longest to shortest edge lengths.

Table 2 below describes the quality of the partitioning into two subgraphs obtained by four algorithms. Quality is measured by the number of edges crossing the partition boundary, where fewer is better. The four algorithms are

1. Spectral -- use the second eigenvector as described above
2. Inertial Partitioning -- coordinate bisection as described in Lecture 20
3. Default Random Circle -- as described in Lecture 20. Recall that this is a randomized algorithm, that involves picking a random circle. The more circles chosen, the better the partitioning (i.e. the fewer edges cut). In this default implementation, a small, fixed number of circles are chosen.
4. Best Random Circle -- In this case circles are repeatedly chosen until no more progress is made. It is more expensive than the Default Random Circle algorithm just described, but gives a better partitioning.

From the table, one sees that the methods are largely comparable, with spectral somewhat better on the largest graphs. (Spectral is also much more expensive to run, although we present no data on this here.) Also, we see that our intuition, that a 2D mesh-like graph with n nodes should have a partition with just sqrt(n) edge crossings, is approximately true. Also, our intuition that a 3D mesh should have n^(2/3) edge crossings is also approximately true.

Mesh	Spectral	Inertial Partitioning	Default Random Circle	Best Random Circle
TAPIR	59	55	37	32
AIRFOIL2	117	172	100	93
TRIANGLE	154	142	144	142
AIRFOIL3	174	230	152	148
PWT	362	562	529	499
BODY	456	953	834	768
WAVE	13706	9821	10377	9773

Table 2: Number of edge crossings for two-way partitions

Finally, we use the partitioning algorithms 7 times recursively in order to partition the graphs into 2^7 = 128 separate partitions, which one would do on a 128-processor machine. Again, the quality of the partitions is largely comparable.

Mesh	Spectral	Inertial Partitioning	Default Random Circle
TAPIR	1278	1387	1239
AIRFOIL2	2826	3271	2709
TRIANGLE	2989	2907	2912

AIRFOIL3	4893	6131	4822
PWT	13495	14220	13769
BODY	12077	22497	19905
WAVE	143015	162833	145155

Table 3: Number of edge crossings for 128-way partitions.

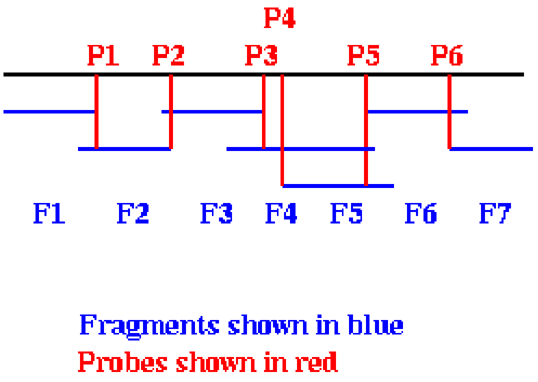
Now we consider coordinate-free algorithms more briefly. According to tests done by Kumar and Karypis, their implementation of multilevel Kernighan-Lin and Leland and Hendrickson's implementation provide partitions of quite similar quality, as does a hybrid multilevel method using both spectral partitioning and Kernighan-Lin. However, theirs is usually twice as fast (or more) s Leland and Hendrickson's, and many times faster than spectral partitioning.

Applying Spectral Ordering to Physical Mapping of DNA

The following material is based on A spectral algorithm for seriation and the consecutive ones problem, by J. Atkins, E. Boman (boman@sccm.stanford.edu) and B. Hendrickson (bahendr@cs.sandia.gov), submitted to SIAM J. of Computing (1995).

Here is a very simple version of the physical mapping problem for DNA. A molecule of DNA is a very long string consisting of a particular sequence of amino acids chosen from a set of four, which may be called A, C, T and G. For example, one might have the sequence ACCTGACTCGAGACTCG, but many millions long. The *sequencing problem* is to determine this sequence for a given molecule of DNA. Current biochemical technology permits the following algorithm to be used. One can break up this long DNA string into a great many shorter *fragments*, which can be separated according to their amino acid sequences. The goal is to represent the original DNA as a sequence of these possibly overlapping fragments in some order. Given the sequences making up each fragment, one then knows the sequence making up the original DNA. To extract this representation in terms of fragments, the following experiments are performed. Each fragment F is allowed to bond to the DNA at a point P where the amino acid sequences match. This point is called a *probe*, and is typically a set of amino acids at one end of the fragment. If the probe is long enough, it will match at a unique point along the DNA. One records this information in a matrix B, which has one row for each fragment and one column for each probe, by putting a 1 at entry (F,P). One can perform the same kind of experiment to see which other fragments bond to fragment F at the same probe P, implying that they overlap. Each such bond between fragment F' and fragment F at probe P is recorded by storing a 1 at location (F',P) of the matrix B. In this way, looping through all the fragments, the matrix B is eventually filled in with ones (and zeros elsewhere), where B(F,P)=1 means that fragment F matches the DNA at probe P. This is shown below, where we have labeled the fragments in sorted order from left to right, and the probes in sorted order from left to right.

DNA Sequencing



$$B = \begin{array}{cccccc|c} P1 & P2 & P3 & P4 & P5 & P6 & \\ 1 & & & & & & F1 \\ 1 & 1 & & & & & F2 \\ & 1 & 1 & & & & F3 \\ & & 1 & 1 & 1 & & F4 \\ & & & 1 & 1 & & F5 \\ & & & & 1 & 1 & F6 \\ & & & & & 1 & F7 \end{array}$$

Notice that when the probes and fragments are sorted, B is a band matrix, or more precisely a *consecutive-ones matrix*, which means that for each row all the ones are consecutive (consecutive-ones matrices are not necessarily band matrices in the usual since, but they often are). In practice, one constructs Bp with probes and fragments in some random order, as shown below. The DNA Sequencing problem is to find the ordering of the rows and ordering of the columns of Bp which expose the underlying band matrix B, because this will say what in what order the fragments appear along the DNA.

DNA Unsequenced

$$Bp = \begin{array}{c|cccccc|c} & P5 & P3 & P2 & P4 & P6 & P1 & \\ \hline & & 1 & 1 & & & & F3 \\ & 1 & & & 1 & & & F5 \\ & & & 1 & & & 1 & F2 \\ & 1 & 1 & & 1 & & & F4 \\ & & & & & 1 & & F7 \\ & & & & & & 1 & F1 \\ & 1 & & & & 1 & & F6 \end{array}$$

If there were no errors in Bp, this could be done by procedure like breadth first search. But in practice, the laboratory procedure for determining entries of Bp is quite error prone, so we need a method for making Bp "close to" a band matrix in some sense. This is where spectral ordering comes in.

Let G=(N,E) be an undirected graph, and L(G) its Laplacian. Let N = N- U N+ be an arbitrary partition of the nodes, and let x be a column vector, where x(i) = +1 if i is in N+, and x(i) = -1 if i is in N-. In Lemma 1 of the last lecture, we showed that the number of edges connecting N+ and N- was equal to

$$.25 * \text{sum}_{\text{edges } e=(i,j)} (x(i) - x(j))^2$$

Therefore, the partition N = N- U N+ which minimizes the number of connecting edges is given by the solution x of the minimization problem

$$\min_{[\ x(i) = +1 \text{ or } -1,\ \text{sum}_i\ x(i) = 0\ ]} \quad .25 * \text{sum}_{\text{edges } e=(i,j)} (x(i) - x(j))^2$$

The spectral partitioning algorithm involved solving the following approximation:

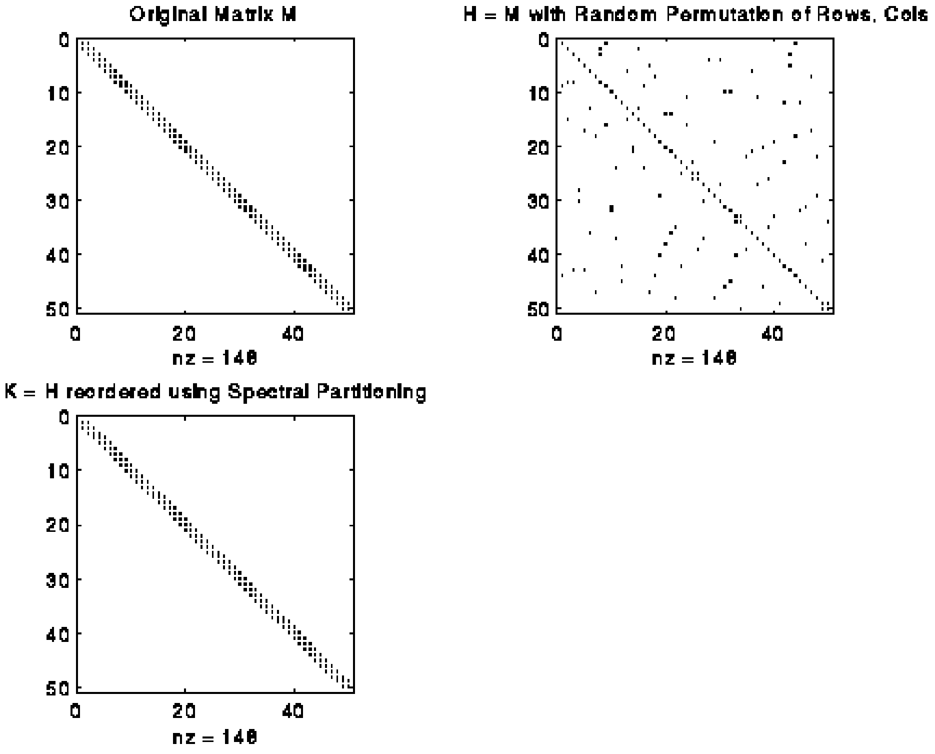
$$\min_{\text{sum\_i } v(i)\text{\^{}}2 = |N|,\ \text{sum\_i } v(i) = 0} \quad .25 * \text{sum}_{\text{edges } e=(i,j)} (v(i) - v(j))^2$$

and then choosing x(i) = sign(v(i)).

One can think of this algorithm as embedding the graph G into the real axis, putting node i at location v(i). If e=(i,j) is an edge, then we draw a line segment from v(i) to v(j), which has length |v(i) - v(j)|. The spectral bisection algorithm chooses this embedding into the real axis so as to minimize the sum of squares of the lengths of these line segments, subject to the constraints sum_i v(i)^2 = |N|, and sum_i v(i)=0.

Suppose we start with a symmetric matrix H, form its graph G(H), and apply the above algorithm, yielding a second eigenvector v of L(G(H)). Let P be a *permutation matrix*, i.e. the identity matrix with its columns permuted, such that the entries of P*v, which are the the entries of v permuted the same way, are in sorted order. Now form K = P*H*P'. K is the matrix H with its rows and columns reordered in the same way that sorts v. The fact that the sum of all (v(i)-v(j))^2 is minimized, means that there are few edges connecting distant v(i) and v(j). In other words, if v(i) and v(j) are widely separated in the sorted list of entries of v, they are unlikely to have an edge connecting them. In the matrix K, this means that there are few nonzero entries far from the diagonal, because these would correspond to an edge from a v(i) to a v(j) widely separated in the sorted list. In other words, K is close to a band matrix.

For example, consider the matrix M = L(G), where G is a chain of n nodes. M is a tridiagonal matrix as shown in the figure below. Now perform a random permutation of the rows and columns of M to get H. H has nonzeros uniformly distributed off the diagonal. Apply spectral partitioning to H as described above to get K. As shown below, K is tridiagonal again. (The label nz under each graph is the number of nonzeros entries in the matrix.)



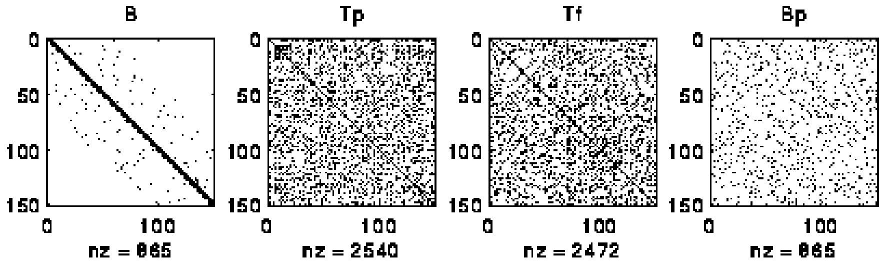
This bandwidth narrowing property (or, more precisely, "consecutive-one-ifying" property) is what we need to reorder the rows and columns of Bp to make it a band (or consecutive-ones) matrix. But reordering Bp requires two permutations, one for the rows and one for the columns, while spectral bisection computes just one permutation. We get around this as follows. We can write Bp = Pf*B*Pp', where Pf and Pp are two unknown permutation matrices we wish to compute; Pf shuffles the rows of B, and Pp shuffles the columns. Now consider the symmetric matrix

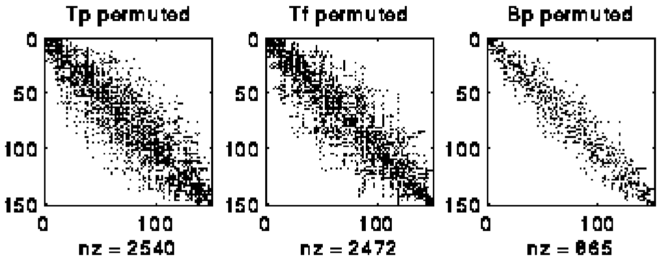
```
Tp = Bp'*Bp = (Pf*B*Pp')'*(Pf*B*Pp') = Pp*(B'*B)*Pp'
```

Note that Tp only depends on Pp and B, but not on Pf. If B is a band matrix, one can confirm that B'*B is too, although with a larger bandwidth. (If B is a consecutive-ones matrix, B'*B shares a similar property; see A spectral algorithm for seriation and the consecutive ones problem for details.) Thus, Pp can be determined just by using spectral bisection to find the single permutation of rows and columns of Tp that makes Pp'*Tp*Pp (nearly) a band matrix. Similarly one can apply spectral bisection to

```
Tf = Bp*Bp' = (Pf*B*Pp')*(Pf*B*Pp')' = Pf*(B*B')*Pf'
```

to independently determine Pf. An example is shown below, where we start with a perfect band matrix and add a few other random entries to get B, and randomly permute its rows and columns to get Bp. The bottom row of three matrices shows Tp, Tf and Bp after permuting them to make them close to band matrices. One can see that the construction is far from "perfect", and in fact degrades more if the random entries added to B are farther from the diagonal. The physical mapping of DNA remains a hard problem.





PARTI: Using Graph Partitioning in a High Level Language

The graph partitioning software described so far, and listed in Lecture 20, consists of libraries to which one passes a graph, and is returned a partitioning. There have also been attempts to embed graph partitioning in a higher level language, so as shield the user from having to construct the graph, partition it, (re)distribute the data across the machine, and set up the communication. The goal of this work is to be able to take an existing serial code which traverses a sparse data structure, and modify the language and compiler to permit the user to say

1. Inspect the following section of code (a loop nest, say), and determine the underlying graph G describing how data items depend on other data items, partition G, and redistribute the data accordingly.
2. Execute the code with the redistributed data.

The system we will describe is called PARTI, and has more recently been renamed CHAOS. This material is taken from "Distributed Memory Compiler Methods for Irregular Problems -- Data Copy Reuse and Runtime Partitioning," by J. Saltz, R. Das, R. Ponnusamy, and D. Mavripilis, ICASE Report 91-73, NASA Langley Research Center, Hampton VA, 1991.

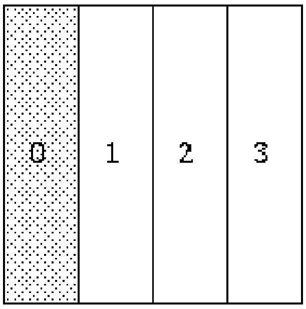
PARTI is an extension of HPF (High Performance Fortran), and uses the features of HPF for describing array layouts across processors. We begin by reviewing data layouts.

At the end of Lecture 5, we discussed data layout in CM Fortran, where for example the declaration (KEYWORDS are capitalized)

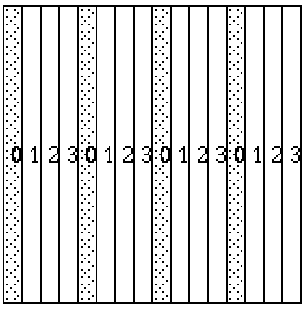
```
      REAL a(64,8), b(64,8), c(64,8)
CMF$  LAYOUT a( :NEWS, :SERIAL ), b( :NEWS, :SERIAL ),
CMF$  LAYOUT c( :SERIAL, :NEWS )
```

indicated that A(i,j) was to be stored in the j-th memory location of processor i, the same for B(i,j), and that C(i,j) was instead to be stored in the i-th memory location of processor j. This would mean that the assignment A=B could occur in parallel without communication, but that A=C would require a great deal of communication.

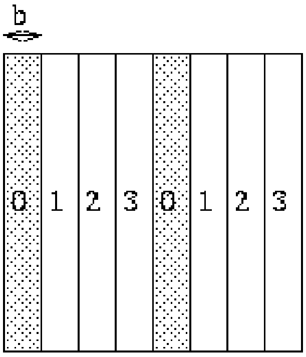
These simple layout directive are not enough for all purposes. In the beginning of Lecture 13, we discussed the more complicated data layouts required to do Gaussian elimination (or other dense linear algebra problems) efficiently on a distributed memory machine, and said the the first four of the following layouts were declarable within the HP Fortran language:



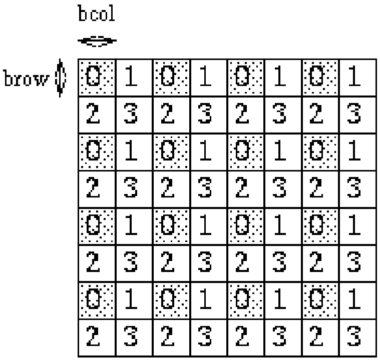
1) Column Blocked Layout



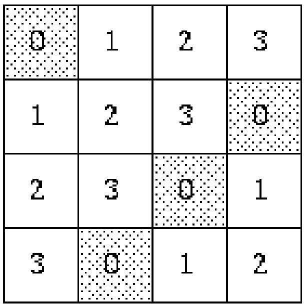
2) Column Cyclic Layout



3) Column Block Cyclic Layout



4) Row and Column Block Cyclic Layout



5) Block Skewed Layout

Here, very briefly, is how HPF permits users to declare these kinds of layouts. Rather than saying how each matrix entry maps to a processor location, two levels of indirection are used. The first level declaration declares how many of the available processors are to be used in the layout. A simple example is the following, which declares mygrid to be a linear array of 4 processors.

```
PROCESSOR mygrid(4)
```

The second level declares a *template*, or "virtual array", and says how to lay it out on mygrid. For example

```
TEMPLATE template_blocked(100),template_cyclic(100)
DISTRIBUTE template_blocked(BLOCK) ONTO mygrid
DISTRIBUTE template_cyclic(CYLIC) ONTO mygrid
```

declares that template_blocked(0:24) is mapped to processor 0, template_blocked(25:49) is mapped to processor 1, and so on, in general with template_blocked(i) mapping to processor floor(i/25). Also, template_cyclic(i) is mapped to processor i mod 4. Block cyclic layouts are also available. Multi-dimensional arrays can have each subscript mapped independently, as preferred for Gaussian Elimination.

A template has no memory allocated for it; it just describes a layout. The final level of declaration actually allocates memory for arrays. For example

```
REAL  a(100), b(100), c(100)
ALIGN a(i) WITH template_block(i)
ALIGN b(i) WITH template_block(i)
ALIGN c(i) WITH template_cyclic(i)
```

declares 3 arrays of 100 entries each. a(i) and b(i) are declared to be stored at the same place as the template entry template_block(i), in this case floor(i/25). However template_block is DISTRIBUTEd, a(i) and b(i) will always be on the same processor. c(i) is declared to be stored at the same place as template_cyclic(i), that is i mod 4.

The reason for these levels of indirection is that one can independently control the amount of parallelism (via PROCESSOR), the layout (via DISTRIBUTE) and which variables are local with which other (via ALIGN).

The same mechanism can be used for more irregular layouts, but we need one more level of indirection to specify the irregularity. For example

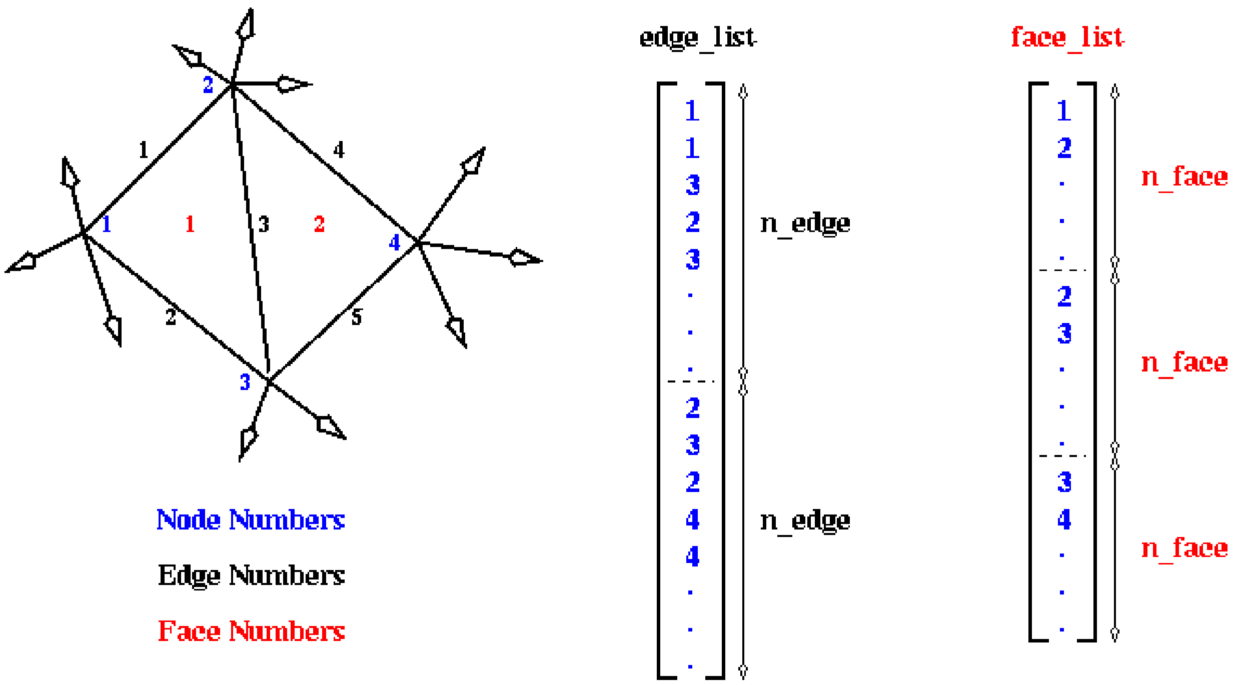
```
TEMPLATE irregular(100)
INTEGER map(100)
DATA map/3,2,2,1,1,1,3,0,1,2,... /
      ... 100 values from 0 to 3
DISTRIBUTE irregular(map) ONTO mygrid
REAL d(100)
ALIGN d(i) WITH irregular(i)
```

These declarations specify that irregular(i) is mapped to processor map(i), i.e. irregular(1) is mapped to processor map(1)=3, irregular(2) is mapped to processor map(2) = 2, and so on. The ALIGN statement in turn says d(1) is stored on processor 3, d(2) is stored on processor 2, and so on.

In this example, map is specified at compile-time, and the decision about where to store d(i) is specified at compile-time. This is very limiting, since we probably won't know the actual data structure we need to partition until run-time. The extensions in PARTI to this approach are to allow map to be computed at run time (by examining some user specified loops and doing graph partitioning), and DISTRIBUTE to be executed at run-time as well, in effect recompiling the code at run-time. This is likely to be quite expensive, and so is done only when the user wants to.

Here is an example, taken from a computational fluid dynamic (CFD) application. The data structure is a two-dimension triangular mesh, made up of nodes (numbered in blue), edges (numbered in black) and faces (numbered in red). The mesh data is stored in two arrays. The edge_list array stores a pair of nodes for each each edge: the nodes numbers for the i-th edge are stored at edge_list(i) and edge_list(i + n_edge), where n_edge is the number of edges. The face_list array stores a triple of nodes for each face: the nodes for the i-th face are stored at face_list(i), face_list(i + n_face), and face_list(i + 2*n_face), as shown below. For example, face 1 has corners at nodes 1, 2 and 3. face 2 at nodes 2, 3 and 4, and so on.

Computational Mesh and Data Structures to Illustrate PARTI



edge_list = list of pairs of node numbers determining each edge

face_list = list of triples of node numbers determining each face

n_node = number of nodes

n_edge = number of edges

n_face = numbers of faces

The original sequential program has two data arrays, x and y, which store data associated with each node. In other words x(i) and y(i) are data about the fluid flow at node i. The algorithm has two loops. Loop L1 below loops over all edges, and for each edge updates the data at both nodes determining that edge. Loop L2 loops over all faces, and for each face updates the data at the three nodes determining the face. The functions foo1, foo2, etc, are simple scalar functions of their scalar arguments, whose details do not concern us.

```
    REAL x(n_node), y(n_node)
    ...
C   Loop over all edges
L1: DO i = 1, n_edge
       n1 = edge_list(i)
       n2 = edge_list(i + n_edge)
       y(n1) = foo1(y(n1),y(n2),x(n1),x(n2))
       y(n2) = foo2(y(n1),y(n2),x(n1),x(n2))
    END DO

C   Loop over all faces
L2: DO i = 1, n_face
       n1 = face_list(i)
       n2 = face_list(i + n_face)
       n3 = face_list(i + 2*n_face)
       y(n1) = foo4(y(n1),...,x(n3))
       y(n2) = foo5(y(n1),...,x(n3))
       y(n3) = foo6(y(n1),...,x(n3))
    END DO
```

Here is the parallel version of this program using PARTI:

```
    REAL x(n_node), y(n_node)
    TEMPLATE coupling(n_node)
    DISTRIBUTE coupling(BLOCK) ONTO mygrid
    ALIGN x(i), y(i) WITH coupling(i)
    ...
C   Decide whether to redistribute data
    IF (time_to_remap) THEN
       DISTRIBUTE coupling(IMPLICIT USING L1)
    END IF
C   Loop over all edges

    IMPLICITMAP(x,y) L1
L1: DO i = 1, n_edge
       n1 = edge_list(i)
       n2 = edge_list(i + n_edge)
       y(n1) = foo1(y(n1),y(n2),x(n1),x(n2))
       y(n2) = foo2(y(n1),y(n2),x(n1),x(n2))
    END DO

C   Loop over all faces
L2: DO i = 1, n_face
       n1 = face_list(i)
       n2 = face_list(i + n_face)
       n3 = face_list(i + 2*n_face)
       y(n1) = foo4(y(n1),...,x(n3))
       y(n2) = foo5(y(n1),...,x(n3))
       y(n3) = foo6(y(n1),...,x(n3))
    END DO
```

Initially, the TEMPLATE coupling is laid out in a blocked fashion onto the processor grid mygrid. Arrays x and y are aligned with coupling. Later, perhaps after the arrays edge_list and face_list have been set up, the user sets time_to_remap to true, and executes the DISTRIBUTE statement following the IF statement. At this point, the system begins the "Inspection phase": It will examine loop L1, which is identified later with the IMPLICITMAP statement. The arguments x and y of IMPLICITMAP tell the system to compute the graph G of data dependencies among the references to x and y in the subsequent loop L1. This is done by executing loop L1 "symbolically", i.e. running through thg loop from i=1 to n_edge, computing the subscripts n1 = edge_list(i) and n2 = edge_list(i + n_edge), seeing that y(n1) depends on y(n1), y(n2), x(n1), and x(n2), and adding nodes n1 and n2, and edge (n1,n2), to graph G, which is initially empty. Functions foo1 and foo2 are not evaluated, and y(n1) and y(n2) are not changed. After computing G, a graph partitioning routine is called to break G into as many pieces as there are processors in mygrid. The partitioning information is stored in the TEMPLATE coupling, with coupling(i) = j if the partition algorithm puts node i onto processor j. All arrays ALIGNed with coupling (namely x and y) are redistributed according to the newly updated coupling. Finally, all parts of the program that reference arrays x or y are "recompiled" to insert the necessary communications to continue to access the data they need.

After completing the "IF (time_to_remap)" block, one reaches loop L1. At this point, the "Execute phase", the newly recompiled code is executed and array y updated. Loop L2 is executed similarly.