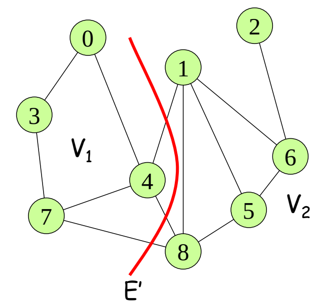
296.3:Algorithms in the Real World

Graph Separators
- Introduction
- Applications

Edge Separators

An *edge separator* :
a set of **edges** $E' \subseteq E$
which partitions V into
V_1 and V_2

Criteria:
$|V_1|$, $|V_2|$ balanced
$|E'|$ is small



Vertex Separators

An *vertex separator* :
a set of **vertices** $V' \subseteq V$
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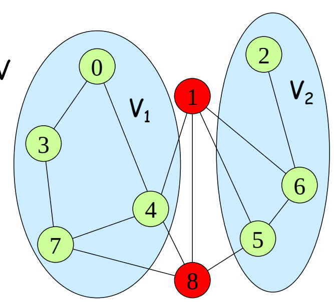


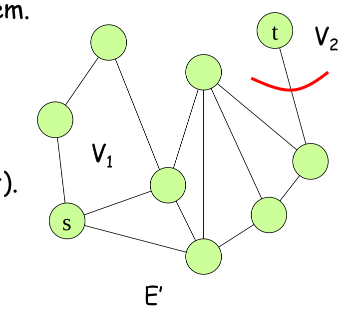
Compared with Min-cut

Min-cut: as in the min-cut, max-flow theorem.

Min-cut has no balance criteria.

Min-cut typically has a source (s) and sink (t).

Min-cut tends to find unbalanced cuts.

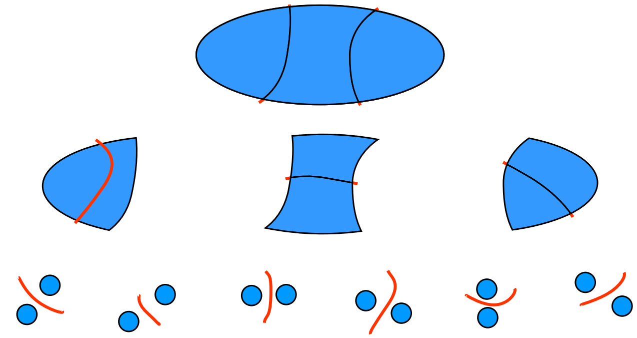


Other names

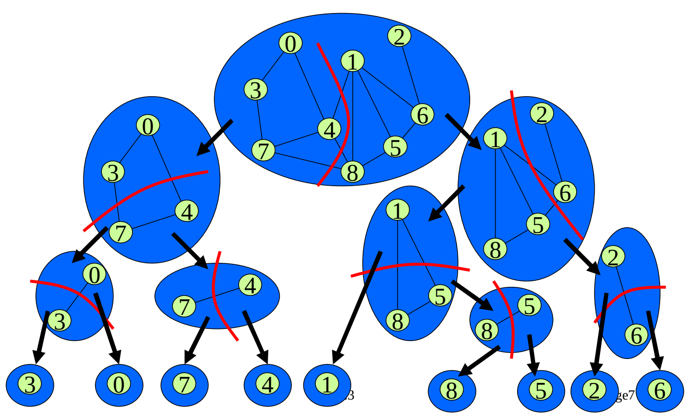
Sometimes referred to as

- **graph partitioning** (probably more common than "graph separators")
- graph bisectors
- graph bifurcators
- balanced or normalized graph cuts

Recursive Separation



Recursive Separation



What graphs have small separators?

Planar graphs: $O(n^{1/2})$ vertex separators

2d meshes, constant genus, excluded minors

Almost planar graphs:

the Internet, power networks, road networks

Circuits

need to be laid out without too many crossings

Social network graphs:

phone-call graphs, link structure of the web, citation graphs, "friends graphs"

3d-grids and meshes: $O(n^{2/3})$

What graphs don't have small separators

Hypercubes:
O(n) edge separators
$O(n/(\log n)^{1/2})$ vertex separators

Butterfly networks:
O(n/log n) separators

Expander graphs:
Graphs such that for any $U \subseteq V$, s.t. $|U| \leq \alpha |V|$, $|\mathbf{neighbors}(U)| \geq \beta |U|$. $(\alpha < 1, \beta > 0)$
random graphs are expanders, with high probability

It is exactly the fact that they don't have small separators that make these graphs useful.

Applications of Separators

Applications of Separators

Circuit Layout (from 1960s)
VLSI layout
Solving linear systems
(nested dissection)
$n^{3/2}$ time for planar graphs
Partitioning for parallel algorithms
Approximations to NP hard problems
TSP, maximum-independent-set
Compact Routing and Shortest-paths
Clustering and machine learning
Machine vision

Out of core algorithms
Register allocation
Shortest Paths
Graph compression
Graph embeddings

Available Software

METIS: U. Minnesota
PARTY: University of Paderborn
CHACO: Sandia national labs
JOSTLE: U. Greenwich
SCOTCH: U. Bordeaux
GNU: Popinet

Benchmarks:
- Graph Partitioning Archive

Different Balance Criteria

Bisectors: 50/50

Constant fraction cuts: e.g. 1/3, 2/3

Trading off cut size for balance (~~vertex~~ edge separators):

min cut criteria: $\min_{V'\subset V}\left(\frac{\cancel{|V'|}\ |E'|}{|V_1||V_2|}\right)$ flux

min quotient separator: $\min_{V'\subset V}\left(\frac{\cancel{|V'|}\ |E'|}{\min(|V_1|,|V_2|)}\right)$ isoperimetric number = sparsity

All versions are NP-hard

Other Variants of Separators

k-Partitioning:
Might be done with recursive partitioning, but direct solution can give better answers.

Weighted:
Weights on edges (cut size), vertices (balance)

Hypergraphs:
Each edge can have more than 2 end points
common in VLSI circuits

Multiconstraint:
Trying to balance different values at the same time.

Asymptotics

If S is a class of graphs closed under the subgraph relation, then

Definition: S satisfies an $f(n)$ vertex-separator theorem if there are constants $\alpha < 1$ and $\beta > 0$ so that for every $G \in S$ there exists a vertex cut set $V' \subseteq V$, with

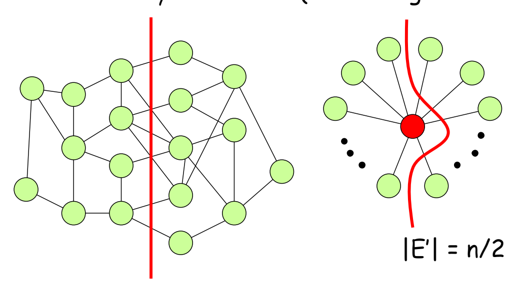
1. $|V'| \leq \beta\ f(|G|)$ cut size
2. $|V_1| \leq \alpha\ |G|$, $|V_2| \leq \alpha\ |G|$ balance

Similar definition for edge separators.

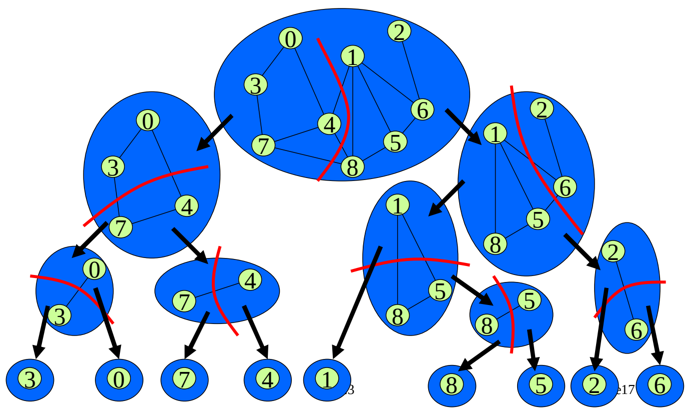
Edge vs. Vertex separators

If a class of graphs satisfies an $f(n)$ edge-separator theorem then it satisfies an $f(n)$ vertex-separator.

The other way is not true (unless degree is bounded)



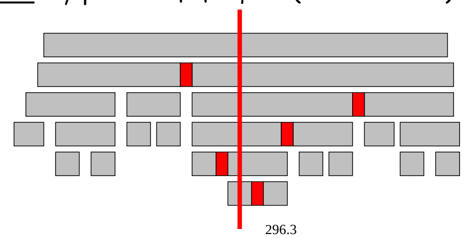
Separator Trees



Separator Trees

Theorem: For S satisfying an (α,β) $f(n) = n^{1-\varepsilon}$ edge-separator theorem, we can generate a perfectly balanced separator with size $|C| \leq k\,\beta\, f(|G|)$.

Proof: by picture $|C| \leq \beta\, n^{1-\varepsilon}(1 + \alpha + \alpha^2 + \ldots) \leq \beta\, n^{1-\varepsilon}(1/1-\alpha)$



Algorithms for Partitioning

All are either heuristics or approximations

- Kernighan-Lin, Fiduccia-Mattheyses (heuristic)
- Planar graph separators
  (finds $O(n^{1/2})$ separators)
- Geometric separators
  (finds $O(n^{(d-1)/d})$ separators in R^d)
- Spectral (finds $O(n^{(d-1)/d})$ separators in R^d)
- Flow/LP-based techniques
  (give log(n) approximations)
- Multilevel recursive bisection
  (heuristic, currently most practical)

Kernighan-Lin Heuristic

Local heuristic for <u>edge-separators</u> based on "hill climbing". Will most likely end in a local-minima.

Two versions:

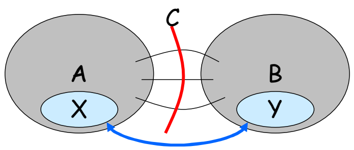
Original K-L: takes n^2 time per pass

Fiduccia-Mattheyses: takes linear time per pass

High-level description for both

Start with an initial cut that partitions the vertices into two equal size sets V_1 and V_2

Want to swap two equal sized sets $X \subset A$ and $Y \subset B$ to reduce the cut size.



Note that finding the optimal subsets X and Y solves the optimal separator problem, so it is NP hard.

We want some heuristic that might help.

Some Terminology

C(A,B) : the weighted cut between A and B

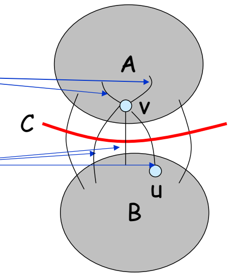
I(v) : the number of edges incident on v that stay within the partition

E(v) : the number of edges incident on v that go to the other partition

D(v) : E(v) - I(v)

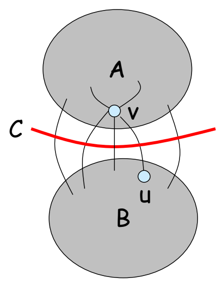
D(u,v) : D(u) + D(v) - 2 w(u,v)

the gain for swapping u and v



Kernighan-Lin improvement step

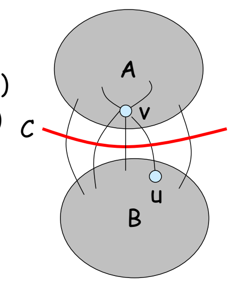
KL(G,A_0,B_0)
 $\forall$ u $\in A_0$, v $\in B_0$
  put (u,v) in a PQ based on D(u,v)
 for k = 1 to |V|/2
  (u,v) = max(PQ)
  $(A_k,B_k) = (A_{k-1},B_{k-1})$ swap (u,v)
  delete u and v entries from PQ
  update D on neighbors (and PQ)
select A_k,B_k with best C_k



Note that can take backward steps ("gain" D(u,v) can be negative).

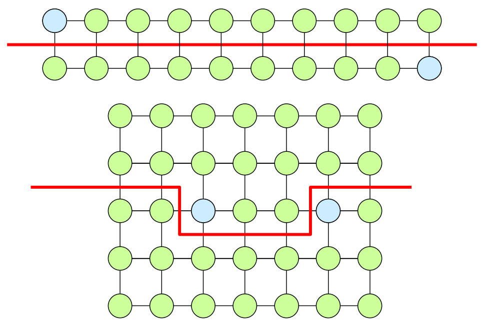
Fiduccia-Mattheyses's improvement step

FM(G,A_0,B_0)
$\forall$ u $\in A_0$ put u in PQ_A based on D(u)
$\forall$ v $\in B_0$ put v in PQ_B based on D(v)
 for k = 1 to |V|/2
  u = max(PQ_A)
  put u on B side and update D
  v = max(PQ_b)
  put v on A side and update D
 select A_k,B_k with best C_k



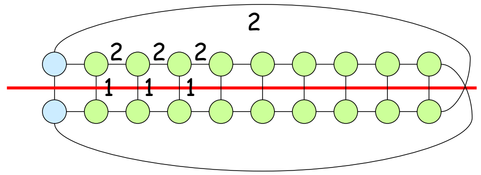
Two examples of KL or FM

Consider following graphs with initial cut given in red.



A Bad Example for KL or FM

Consider following graph with initial cut given in red.



KL (or FM) will start on one side of the grid (e.g. the blue pair) and flip pairs over moving across the grid until the whole thing is flipped.

After one round the graph will look identical?

Boundary Kernighan-Lin (or FM)

Instead of putting all pairs (u,v) in Q (or all u and v in Q for FM), just consider the boundary vertices (i.e. vertices adjacent to a vertex in the other partition).

Note that vertices might not originally be boundaries but become boundaries.

In practice for reasonable initial cuts this can speed up KL by a **large** factor, but won't necessarily find the same solution as KL.

Performance in Practice

In general the algorithms do very well at smoothing a cut that is approximately correct.

Works best for graphs with reasonably high degree.

Used by most separator packages either

1. to smooth final results
2. to smooth partial results during the algorithm

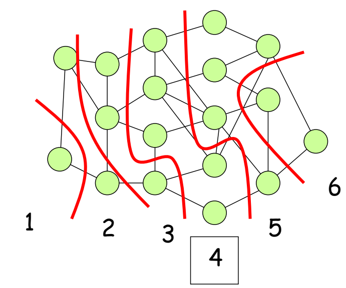
Separators Outline

Introduction:

Algorithms:

- **Kernighan Lin**
- **BFS and PFS**
- **Multilevel**
- **Spectral**
- LP-based

Breadth-First Search Separators



Run BFS and as soon as you have included half the vertices return that as the partition.

Won't necessarily be 50/50, but can arbitrarily split vertices in middle level.

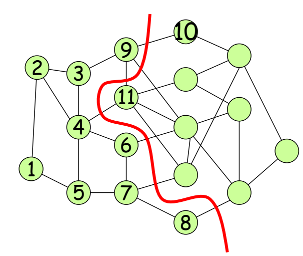
Used as substep in Lipton-Tarjan planar separators.

In practiced does not work well on its own.

Picking the Start Vertex

1. Try a few random starts and select best partition found
2. Start at an "extreme" point.
   Do an initial DFS starting at any point and select a vertex from the last level to start with.
3. If multiple extreme points, try a few of them.

Priority-First Search Separators



Prioritize the vertices based on their gain (as defined in KL) with the current set.

Search until you have half the vertices.

Multilevel Graph Partitioning

Suggested by many researchers around the same time (early 1990s).

Packages that use it:

- METIS
- Jostle
- TSL (GNU)
- Chaco

Best packages in practice (for now), but not yet properly analyzed in terms of theory.

Mostly applied to edge separators.

High-Level Algorithm Outline

MultilevelPartition(*G*)

If *G* is small, do **something brute force**

Else

Coarsen the graph into *G'* (Coarsen)

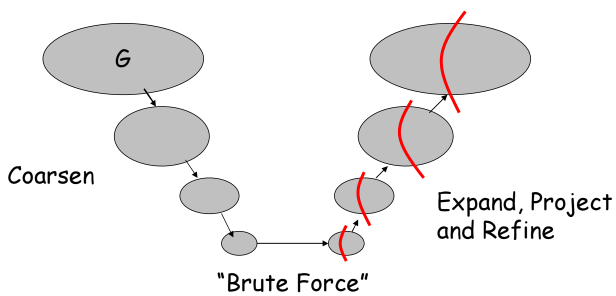
A',B' = MultilevelPartition(*G'*)

Expand graph back to *G* and **project** the partitions A' and B' onto A and B

Refine the partition A,B and return result

Many choices on how to do underlined parts

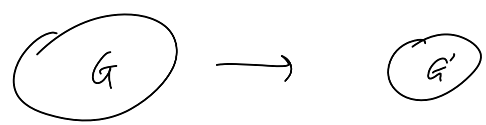
MGP as Bubble Diagram



How to Coarsen

Goal is to pick a sample *G'* such that when we find its partition it will help us find the partition of *G*.

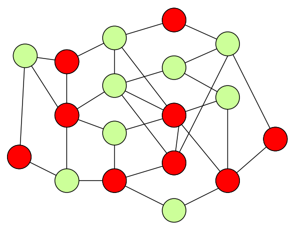
Possibilities?



(a) hierarchical clustering — clustering using cliques

(b) randomly select

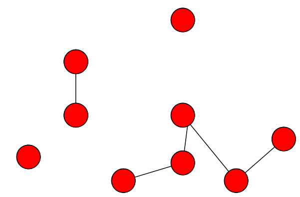
Random Sampling



Pick a random subset of the vertices.

Remove the unchosen vertices and their incident edges

Random Sampling



Pick a random subset of the vertices.

Remove the unchosen vertices and their incident edges

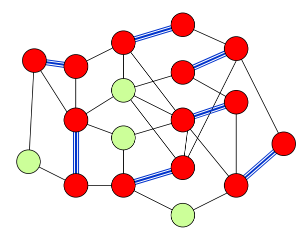
Graph falls apart if it is not dense enough.

Maximal Matchings

A maximal matching is a pairing of neighbors so that no unpaired vertex can be paired with an unpaired neighbor.

The idea is to contract pairs into a single vertex.

A Maximal Matching

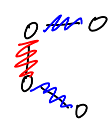


$M \subseteq E$ is a matching

M is maximal

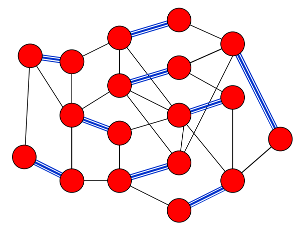
if $\nexists\, M' \supseteq M$

M' is a matching as well.



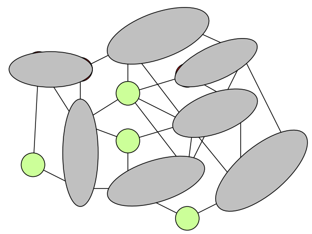
Can be found in linear time greedily.

A side note

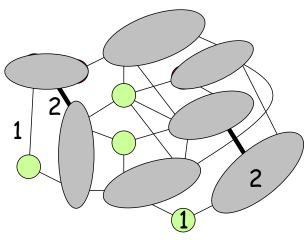


Compared to a **maximum** matching: a pairing such that the number of covered nodes is maximum

Coarsening



Collapsing and Weights



Why care about weights?

New vertices become weighted by sum of weights of their pair.

New edges (u,v) become weighted by sum of weights of multiple edges (u,v)

We therefore have to solve the weighted problem.

Heuristics for finding the Matching

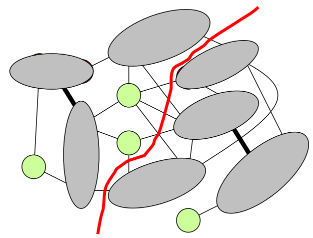
Random : randomly select edges.

Prioritized: the edges are prioritized by weight. Visit vertices in random order, but pick highest priority edge first.

- **Heaviest first:** Why might this be a good heuristic?
- **Lightest first**: Why might this be a good heuristic?

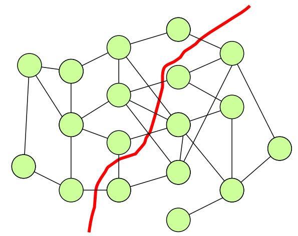
Highly connected components: (or heavy clique matching). Looks not only at two vertices but the connectivity of their own structure.

Finding the Cut on the Coarsened Graph



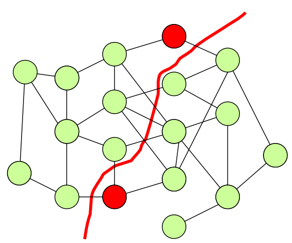
296.3 Page45

Exanding and "Projecting"



296.3 Page46

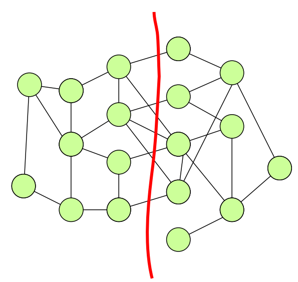
Refining



e.g. by using
Kernighan-Lin

296.3 Page47

After Refinement



296.3 Page48

METIS

Coarsening: "Heavy Edge" maximal matching.

Base case: Priority-first search based on gain. Randomly select 4 starting points and pick best cut.

Smoothing: Boundary Kernighan-Lin

Has many other options. e.g., Multiway separators.

Separators Outline

Introduction:

Algorithms:

- **Kernighan Lin**
- **BFS and PFS**
- **Multilevel**
- **Spectral**

Spectral Separators

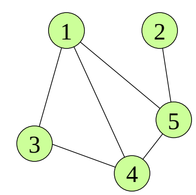
Based on the second eigenvector of the "Laplacian" matrix for the graph.

Let **A** be the adjacency matrix for G.

Let **D** be a diagonal matrix with degree of each vertex.

The **Laplacian** matrix is defined as **L = D-A**

Laplacian Matrix: Example



$$L = \begin{pmatrix} 3 & 0 & -1 & -1 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ -1 & 0 & 2 & -1 & 0 \\ -1 & 0 & -1 & 3 & -1 \\ -1 & -1 & 0 & -1 & 3 \end{pmatrix}$$

Note that each row sums to 0.

Fiedler Vectors

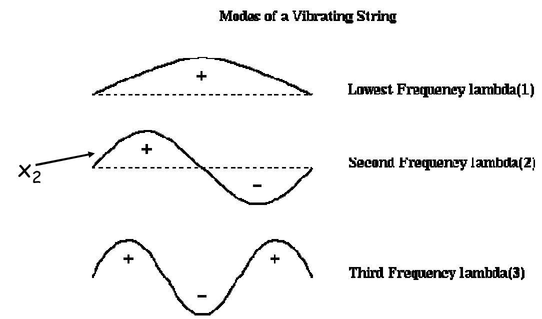
Eigenvalues $\lambda_1 \leq \lambda_2 \leq \lambda_3 \leq \ldots \leq \lambda_n$, real, non-negative.

Find eigenvector corresponding to the second smallest eigenvalue: $L\, x_2 = \lambda_2\, x_2$

This is called the **Fiedler** vector.

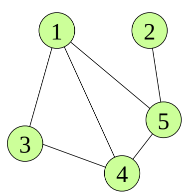
What is true about the first eigenvector?

Modes of Vibration



(Picture from Jim Demmel's CS267 course at Berkeley.)

Fiedler Vector: Example



$$L = \begin{pmatrix} 3 & 0 & -1 & -1 & -1 \\ 0 & 1 & 0 & 0 & -1 \\ -1 & 0 & 2 & -1 & 0 \\ -1 & 0 & -1 & 3 & -1 \\ -1 & -1 & 0 & -1 & 3 \end{pmatrix} \quad x_2 = \begin{pmatrix} -.26 \\ .81 \\ -.44 \\ -.26 \\ .13 \end{pmatrix}$$

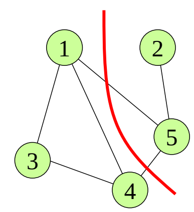
$$Lx_2 = .83 x_2$$

Note that each row sums to 0.

If graph is not connected, what is the second eigenvalue?

Finding the Separator

Sort Fiedler vector by value, and split in half.



$$x_2 = \begin{pmatrix} -.26 \\ .81 \\ -.44 \\ -.26 \\ .13 \end{pmatrix}$$

sorted vertices: [3, 1, 4, 5, 2]

Power Method

Iterative method for finding first few eigenvectors.

Every vector is a linear combination of its eigenvectors $\mathbf{e}_1, \mathbf{e}_2, \ldots$

Consider: $\mathbf{p}_0 = \mathbf{a}_1\,\mathbf{e}_1 + \mathbf{a}_2\,\mathbf{e}_2 + \ldots$

Iterating $\mathbf{p}_{i+1} = \mathbf{A}\mathbf{p}_i$ until it settles will give the principal eigenvector (largest magnitude eigenvalue) since

$\mathbf{p}_i = \lambda_1^i\,\mathbf{a}_1\,\mathbf{e}_1 + \lambda_2^i\,\mathbf{a}_2\,\mathbf{e}_2 + \ldots$

(Assuming all a_i are about the same magnitude)

The more spread in first two eigenvalues, the faster it will settle (related to the rapid mixing of expander graphs)

The second eigenvector

Assuming we have the principal eigenvector, after each iteration remove the component that is aligned with the principal eigenvector.

$\mathbf{n}_i = A\,\mathbf{p}_{i-1}$

$\mathbf{p}_i = \mathbf{n}_i - (\mathbf{e}_1 \bullet \mathbf{n}_i)\mathbf{e}_1$ (assuming $\mathbf{e}_1$ is normalized)

Now

$\mathbf{p}_i = \lambda_2^i\,\mathbf{a}_2\,\mathbf{e}_2 + \lambda_3^i\,\mathbf{a}_3\,\mathbf{e}_3 + \ldots$

Can use random vector for initial $\mathbf{p}_0$

Power method for Laplacian

To apply the power method we have to shift the eigenvalues, since we are interested in eigenvector with eigenvalue closest to zero.

How do we shift eigenvalues by a constant amount?

Lanczos' algorithm is faster in practice if starting from scratch, but if you have an approximate solution, the power method works very well.

Multilevel Spectral

MultilevelFiedler(*G*)
- If *G* is small, do **something brute force**
- Else
  - **Coarsen the graph** into *G'*
  - e'_2 = MultilevelFiedler(*G'*)
  - Expand graph back to *G* and **project** e'_2 onto e_2
  - **Refine e_2** using power method and return

To project, you can just copy the values in location i of e'_2 into both vertices i expands into.

This idea is used by Chaco.