A gentle introduction to community detection

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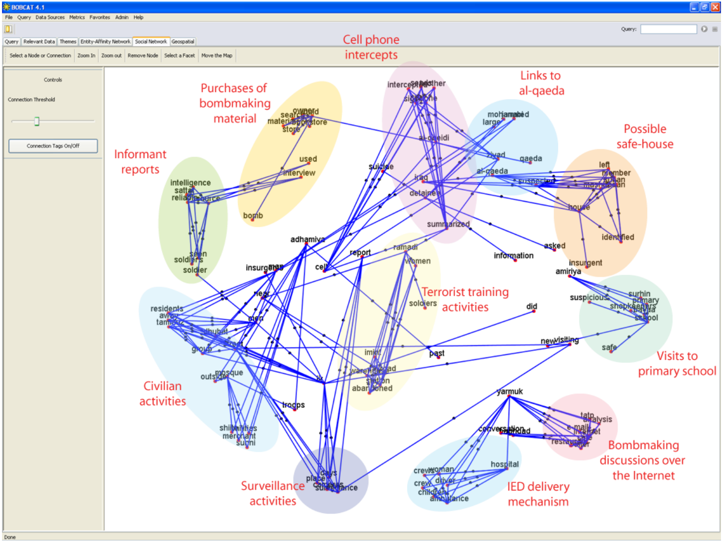
Outline

What is community detection?



Source: `http://www.prweb.com/releases/stopterrorism/bobcatrelease41/prweb711224.htm`

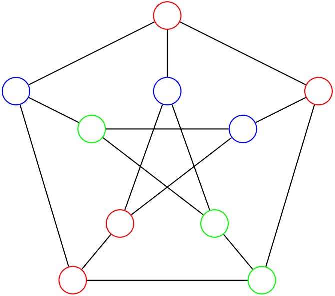
What is community detection?

Goal *Quantitatively* define a community

Hope The *quantitative* definition captures the *qualitative* objective you have in mind

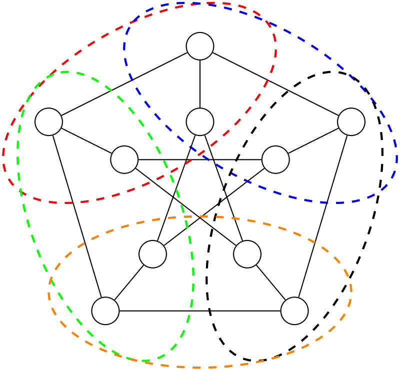
Difficulty Clustering is not a well-defined problem.
Metrics are usually problem specific.
Most clustering formulations are NP-hard

Partitions vs. Covers



- Partition: No overlap. Each vertex only belong to 1 group
- Cover: Overlaps allowed. Can have multiple membership
- Union of either gives us all the vertices
- For this talk, will focus on partition

Partitions vs. Covers



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What do we need?

- A graph - n vertices, m edges
  - Unweighted graph: Sparse
  - Weighted graph: Weights cannot be too homogeneous
- Some concept of measure (see examples below)
  - Local measure: "Goodness" of a cluster
  - Global measure: "Goodness" of an overall partitioning
- For some algorithms,
  - Number of clusters k
  - A threshold value d

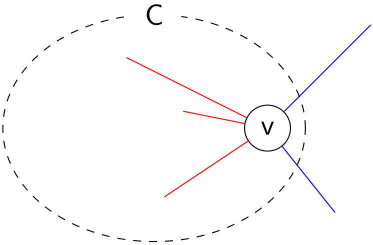
A possible classification of different approaches

Local Form maximal groups that maintain a certain property (e.g. variants of cliques)

Global Maximise global partition based on a criteria (e.g. modularity)

Vertex similarity Group vertices based on how similar they are with respect to certain feature(s)
(e.g. distance in point cloud representation)

Degree and cluster density



- For a vertex v in cluster C, $deg(v) = int_v^C + ext_v^C$
- For a cluster C with n_c vertices,
  - $int^C = \sum_{v \in C} int_v^C$ and $ext^C = \sum_{v \in C} ext_v^C$
  - Intra-cluster density $\delta_{int}(C) = \frac{int^C}{\binom{n}{2}}$
  - Inter-cluster density $\delta_{ext}(C) = \frac{ext^C}{n_c \cdot (n - n_c)}$
- Intuitively, a cluster *should* be a set of vertices with high intra-cluster density and low inter-cluster density

Quality function

- Evaluate 'goodness' of a partition: $Q(\text{Partition}) \rightarrow$ Value
- Most popular: Modularity
  - $Q = \frac{1}{2m} \sum_{v_i, v_j \in V} (A_{i,j} - \frac{deg(v_i) deg(v_j)}{2m}) \mathbb{1}\{v_i \text{ and } v_j \text{ same cluster}\}$
    A = Adjacency matrix
  - Compare partitioning in actual graph against a null model (randomly distribute edges).
  - Higher modularity value $\Rightarrow$ Better community structure (?)

The plan for today

- Graph partitioning (Kernighan-Lin, Spectral bisection)
- Hierarchical clustering (Agglomerative, Divisive)
- Partitional clustering (k-means)
- Spectral clustering

Due to time constraint,

- Details and examples only for some methods
- We can discuss in-depth after the talk :)

Graph partitioning

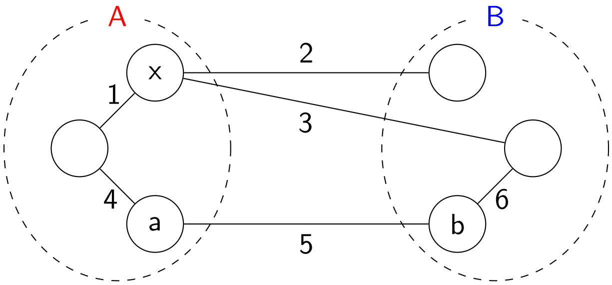
Goal Cut up the graph into 2 parts

Pros Can be efficient and fast

Cons Not natural to always cut into 2.
Need to know number of clusters k

Some methods can be extended to allow multiple cluster cuts, but those methods have poorer run time.

Kernighan-Lin (1970)



- For now, consider only single element swaps[1]
- Gain of moving element x (e.g. from A to B):
  $D(x) = \sum_{(u,x)\in A} w(u,x) - \sum_{(v,x)\in B} w(v,x) = 2 + 3 - 1 = 4$
- Gain of swapping 2 items (e.g. $a \in A, b \in B$): $D(a,b) = D(a) + D(b) - 2 * w(a,b) = (5-4) + (5-6) - 2*(5) = -10$

[1] In general, works with any subset size. Larger subsets $\Rightarrow$ slower run time

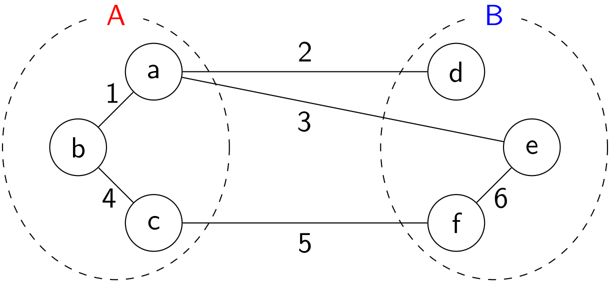
Kernighan-Lin (1970)

Algorithm 1 Kernighan-Lin(G = (V,E))

Initialise partitions A and B
loop ▷ Store copy of originals A, B somewhere
  for $i = 1, \ldots, n$ **do** ▷ Modify working copies of A and B
    Compute $D(x)$ for all $x \in V$
    $a, b \leftarrow \text{argmax}_{a \in A, b \in B}\{D(a, b)\}$ ▷ Swap a and b
    $S[i] \leftarrow (a, b), g[i] \leftarrow D(a, b)$ ▷ Record for later
  end for
  if $\text{argmax}_k \sum_{i=1}^{k} g[i] > 0$ **then** ▷ Best prefix changes
    Permanently apply changes $S[1], \ldots, S[k]$ to originals
  else
    return A, B
  end if
end loop

Kernighan-Lin (1970) tracing: 1/4

Cut size $= 2 + 3 + 5 = 10$



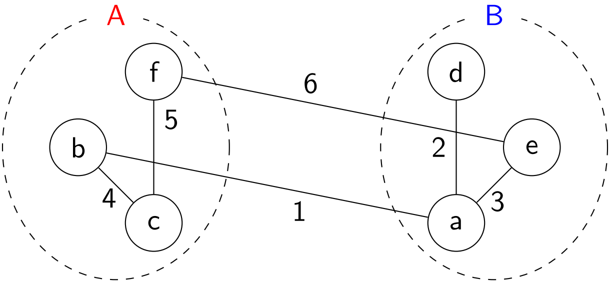
$D(a) = 4$
$D(b) = -5$
$D(c) = 1$

$D(d) = 2$
$D(e) = -3$
$D(f) = -1$

$D(a, f) = 3$ is the largest $\rightarrow$ Swap a and f

Kernighan-Lin (1970) tracing: 2/4

Cut size = 6 + 1 = 7



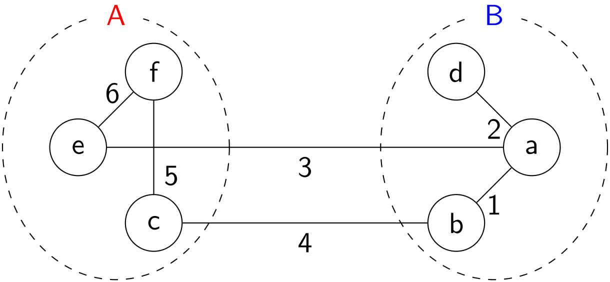
$D(f) = -2$
$D(b) = -3$
$D(c) = -9$

$D(d) = -2$
$D(e) = 3$
$D(a) = -4$

$D(b, e) = 0$ is the largest $\rightarrow$ Swap b and e

Kernighan-Lin (1970) tracing: 3/4

Cut size = 3 + 4 = 7



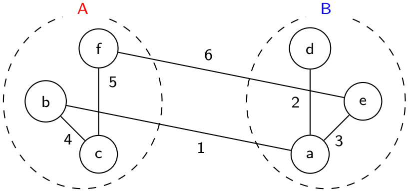
$D(f) = -11$
$D(e) = -3$
$D(c) = -1$

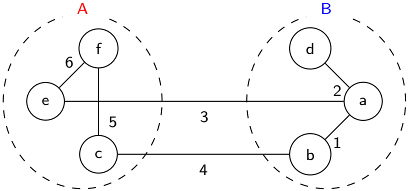
$D(d) = -2$
$D(a) = 0$
$D(b) = -3$

$D(b, e) = -1$ is the largest → Swap a and c

Kernighan-Lin (1970) tracing: 4/4

- Since $D(a, f) = 3$, $D(b, e) = 0$, and $D(b, e) = -1$, the best prefix sum gives us either the 2^{nd} or 3^{rd} graph
- Both yield cut size of 7





Spectral bisection

- (Unnormalized) Laplacian matrix $L = D - A$
  D = diagonal degree matrix
  A = adjacency matrix
- If G is connected, smallest eigenvector λ_1 of L is 0
- Fiedler vector (1973):
  Eigenvector V_2 corresponding to 2^{nd} smallest eigenvalue λ_2
- Bi-partition using Fiedler vector by
  - Sign of values in V_2 (positive vs. negative)
  - Average of values in V_2 (above vs. below average)

Demo

See IPython notebook

Hierarchical clustering

Goal Given a vertex/cluster similarity metric, iteratively join or split up vertices

Pros Do not assume k

Cons Hierarchy may not be natural.
Similarity computation may be expensive

Dendrogram is a useful way of visualising outputs of hierarchical clustering methods.

For a suitable metric f

Agglomerative (Bottom-up):

1. Initialise every vertex as own cluster
2. Compute $f(i,j)$ for clusters i and j (may set $-\infty$ if no edge)
3. Combine clusters $\text{argmax}_{(i,j)} f(i,j)$ with highest f score.
4. Repeat previous 2 steps until only 1 cluster remain

Divisive (Top-down):

1. Compute $f(\cdot)$ for all edges
2. Remove $\text{argmax}_e f(e)$. Handle ties randomly
3. Repeat previous steps until no more edges

Quality of split depends on f, but f cannot be too expensive!

Agglomerative (Bottom-up)

Ways to combine clusters C_1 and C_2:

- Single-linkage (min):

$$f(C_1, C_2) = \min_{i \in C_1, j \in C_2} f(i, j)$$

- Complete-linkage (max):

$$f(C_1, C_2) = \max_{i \in C_1, j \in C_2} f(i, j)$$

- Average-linkage (avg):

$$f(C_1, C_2) = \frac{1}{|C_1| \cdot |C_2|} \sum_{i \in C_1, j \in C_2} f(i, j)$$

Divisive (Top-down)

One popular algorithm: Girvan and Newman (2002)

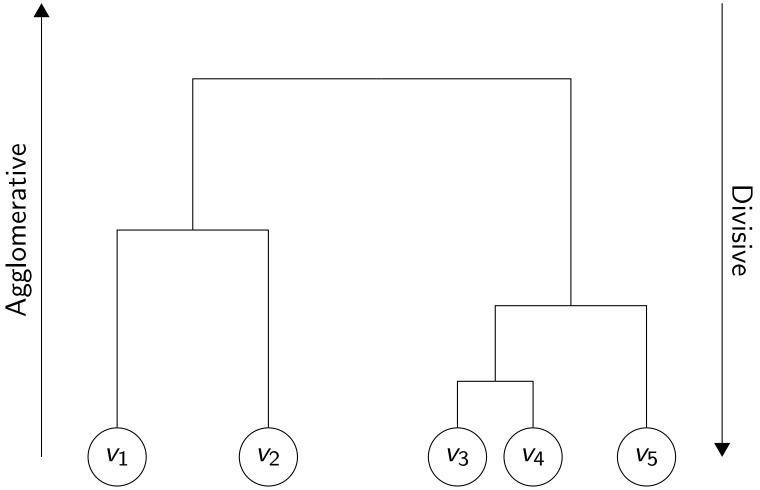
- Lots of modifications and extensions
- Their metric f is the concept of *betweenness*
  Roughly: How frequent an edge is involved in "some process"

3 variants of edge betweenness

1. $f_1(e)$: Geodesic edge betweenness
   \# shortest paths between all vertex pairs that include edge e
2. $f_2(e)$: Random-walk edge betweenness
   How likely is e involved in a random walk from s to t?
3. $f_3(e)$: Current-flow edge betweenness
   Put voltage across 2 vertices $\rightarrow$ Kirchoff's equations.
   $f_3(e) =$ Average current of e across all vertex pairs.

Equations of f_2 and f_3 shown to be equivalent.

Dendrogram example



Partitional clustering

Goal Given a distance metric, separate vertices into clusters based on some cost function involving distances between points in a cluster, or points to a cluster centroid

Pros Fast convergence

Cons Need to know k. Sensitive to initialisation

k-means

Iteratively improve from random initialisation of k centroids

1. Assign vertex to closest centroid
2. Update centroid to average coordinate of all assigned vertices
3. Repeat previous steps until convergence

- A special case of Expectation-Maximisation (EM) algorithms
- Multiple ways to define convergence (can be a mixture):
  - Fixed number of iterations
  - Assignments to clusters did not change
  - Clusters did not change positions
  - Decrease in the sum of distances from vertices to assigned centroids is below a threshold

Demo

See IPython notebook

Spectral clustering

Goal Using a similarity metric, partition sets into clusters using eigenvectors of matrices

Pros Induced metric space tends to reveal clustering properties better

Cons Computation of eigenvalues and eigenvectors may be expensive for large graphs

- Strongly related to perturbation theory, graph cuts, etc.
- Can view as a non-linear graph transformation / dimension-reduction preprocessing step before executing standard techniques like k-means
- Unnormalised Laplacian matrix $L = D - A$ (Fiedler)
- Symmetric normalised Laplacian matrices $L = I - D^{-\frac{1}{2}} A D^{-\frac{1}{2}}$ (Andrew Ng, Michael Jordan, Yair Weiss, etc.)

Spectral clustering with unnormalised Laplacian

1. Compute eigenvectors and eigenvalues of Laplacian $L = D - A$
2. Pick $k = \text{argmax}_{i=2,3,...,n} |\lambda_i - \lambda_{i-1}|$
3. Graph transformation:
   Form new matrix $M = (V_1, V_2, ..., V_k) \in \mathbb{R}^{nxk}$
4. Run k-means on M, treating each row as a point
5. Cluster original points according to k-means results on M

Demo

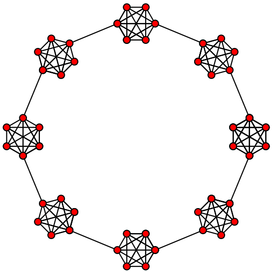
See IPython notebook

Modularity

- Popularised by Newman and Girvan
- Recall modularity: $Q = \frac{1}{2m} \sum_{v_i, v_j \in V} (A_{i,j} - \frac{deg(v_i)deg(v_j)}{2m}) \mathbb{1}\{v_i \text{ and } v_j \text{ same cluster}\}$
- Assumption: Higher $Q \Rightarrow$ Better partition
- Optimize Q to find best partition via methods like greedy agglomeration, simulated annealing, etc.
- Caveat:
  - The assumption doesn't always hold
  - *"Modularity maximum of a graph reveals a significant community structure only if it is appreciably larger than the modularity maximum of random graphs of the same size and expected degree sequence."*
  - See survey paper, Section IV. C. 'Limits of modularity'

Dynamic methods

- Spin models
  - Popular model in statistical mechanics: Potts model
  - Each vertex can hold a different state/spin
  - Goal: Minimise energy $\mathcal{H}$ based on neighbour interactions
- Random walk
  - Community structures have high density of internal edges
  - Random walkers spend long time within the same community



Note: Not dynamic in the sense of a changing graph

Statistical inference methods

- Find best hypothesis that fits actual graph topology
- Bayes theorem: $P(\Theta|D) = \frac{1}{Z}P(D|\Theta)P(\Theta)$
  Θ: Parameters/hypothesis
  D: Data/Actual graph
  Z: Normalizing constant (usually hard to compute)
- Methods usually find Θ that maximise $P(D|\Theta)$.
- Example: Planted partition model (Hastings, 2006)

Planted partition model (Hastings, 2006)

Input Graph G, number of clusters k, p_{in} and p_{out}

Solve $\text{argmax}_{\text{partition } q_i} P(G|q_i)$ via belief propagation

Output Most likely partition q^*

- p_{in}: Probability that vertices in same group are linked
- p_{out}: Probability that vertices in different groups are linked
- Notice similarity to spin model approach.

What's next?

Today:

- Graph partitioning:
  Kernighan-Lin, Spectral bisection via Fiedler vector
- Hierarchical clustering
  Agglomerative, Divisive (Girvan and Newman)
- Partitional clustering: k-means
- Spectral clustering with unnormalised Laplacian

Other interesting directions:

- Finding covers (e.g. clique percolation)
- Multiresolution and cluster hierarchy
- Detection of dynamic communities

How to develop a clustering algorithm?

No single best algorithm for all problem settings.

- Make good observations in your problem domain: Construct and study a few graphs, extract insights, etc.
- Formalise the observation quantitatively
- Find ways to optimise
- Test and check that your *quantitative* measure correctly reflects your *qualitative* goal

Further reading

- Community detection in graphs

  https://arxiv.org/pdf/0906.0612v2.pdf

- A Tutorial on Spectral Clustering

  https://arxiv.org/pdf/0711.0189v1.pdf

- On Spectral Clustering: Analysis and an Algorithm

  http://ai.stanford.edu/~ang/papers/nips01-spectral.pdf