An introduction to graph analysis and modeling
Descriptive Analysis of Network Data

MSc in Statistics for Smart Data – ENSAI

Autumn semester 2017

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Outline

Outline

References

- Statistical Analysis of Network Data: Methods and Models,
  Eric Kolazcyk
  Chapter 2, Section 1
- Analyse statistique de graphes,
  Catherine Matias
  Chapitre 1

Outline

Graphs, Networks: some definitions

Definition (Network versus Graph)

- A Network is a collection of interacting entities
- A Graph is the mathematical representation of a network

Definition (Graph)

A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is a mathematical structure consisting of

- a set $\mathcal{V} = \{1, \ldots, n\}$ of vertices or nodes
- a set $\mathcal{E} = \{e_1, \ldots, e_p : e_k = (i_k, j_k) \in (\mathcal{V} \times \mathcal{V})\}$ of edges or links
- The number of vertices $N_v = |\mathcal{V}|$ is called the order
- The number of edges $N_e = |\mathcal{E}|$ is called the size

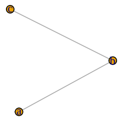
Graphs, Networks: some vocabulary

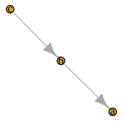
Not comprehensive

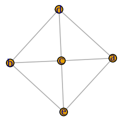
- subgraph $\mathcal{H} = (\mathcal{V}_{\mathcal{H}}, \mathcal{E}_{\mathcal{H}})$,
- induced subgraph
- (un)directed graph,
- weighted graph,
- bipartite graph,
- tree,
- DAG, etc.

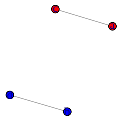
Examples

Undirected, directed (digraph), complete, bipartite









Paths, Cycles, Connected Components I

Definition (Path)

In a undirected graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ a path between $i, j \in \mathcal{V}^2$ is a series of edges $e_1, \ldots, e_k$ such that

- $\forall 1 \leq \ell < k$, all edges $(e_\ell, e_{\ell+1})$ share a vertex in $\mathcal{V}$
- e_1 starts from i, e_k ends to j.

Vocabulary

- A cycle is a path from i to itself.
- A connected component is a subset $\mathcal{V}' \subset \mathcal{V}$ such that there exists an path between any $i, j \in \mathcal{V}'$.
- A graph is connected when there is a path between every pairs of vertices.

Paths, Cycles, Connected Components II

Proposition (Decomposition)

Any graph can be decomposed in a unique set of maximal connected components. The number of connected component is a least $n - |\mathcal{E}|$

Neighborhood, Degree

Definition (Neighborhood)

The neighbors of a vertex are the nodes directly connected to this vertex:

$$\mathcal{N}(i) = \{j \in \mathcal{V} : (i,j) \in \mathcal{E}\}\,.$$

Definition (Degree)

The degree d_i of a node i is given by its number of neighbors, i.e. $|\mathcal{N}(i)|$.

Remark

In digraphs, vertex degree is replaced by in-degree and out-degree.

Proposition

In a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ the sum of the degree is given by $2|\mathcal{E}|$. Hence this is always an even quantity.

Outline

Adjacency matrix and list of edges

Definition (Ajacency matrix)

The connectivity of $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is captured by the $|\mathcal{V}| \times |\mathcal{V}|$ matrix $\mathbf{A}$:

$$(\mathbf{A})_{ij} = \begin{cases} 1 & \text{if } i \sim j, \\ 0 & \text{otherwise.} \end{cases}$$

Proposition

The degree of $\mathcal{G}$ are then simply obtained as the row-wise and/or column-wise sums of $\mathbf{A}$.

Remark

If the list of vertices is known, the only information which needs to be stored is the list of edges. In terms of storage, this is equivalent to a sparse matrix representation.

Incidence matrix

Definition (Incidence matrix)

The connectivity of $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is captured by the $|\mathcal{V}| \times |\mathcal{E}|$ matrix $\mathbf{B}$:

$$(\mathbf{B})_{ij} = \begin{cases} 1 & \text{if } i \text{ is incident to edge } j, \\ 0 & \text{otherwise.} \end{cases}$$

Proposition (Relationship)

Let $\tilde{\mathbf{B}}$ be a modified signed version of $\mathbf{B}$ where $\tilde{B}_{ij} = 1/-1$ if i is incident to j as tail/head. Then

$$\tilde{\mathbf{B}}\tilde{\mathbf{B}}^\intercal = \mathbf{D} - \mathbf{A},$$

where $\mathbf{D} = diag(\{d_i, i \in \mathcal{V}\})$ is the diagonal matrix of degrees.

$\leadsto$ $\tilde{\mathbf{B}}\tilde{\mathbf{B}}^\intercal$ is called the Laplacian matrix and will be studied latter.

Layout and Vizualization

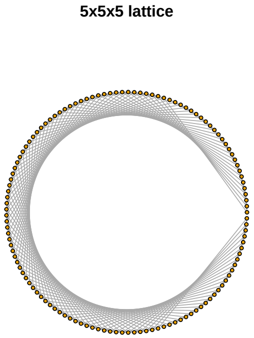
- Vizualization of large networks is a field of research in its own
- Be carefull with graphical interpretation of (large) networks

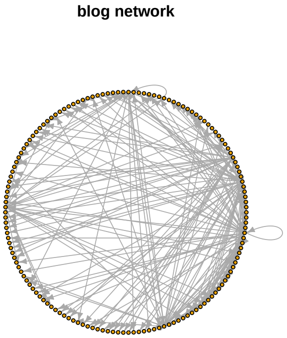
```
library(igraph)
library(sand)
GLattice <- graph.lattice(c(5,5,5))
GBlog <- aidsblog
```

Layout and Vizualization

Example with circle plot

```r
par(mfrow=c(1,2))
plot(GLattice, layout=layout.circle); title("5x5x5 lattice")
plot(GBlog , layout=layout.circle); title("blog network")
```

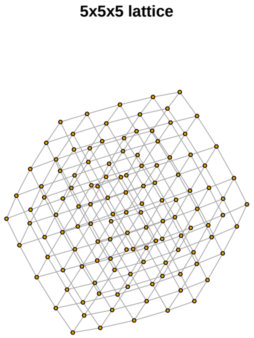


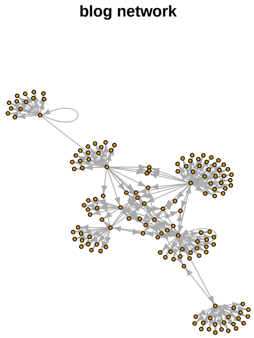


Layout and Vizualization

Example with Fruchterman and Reingold

```
par(mfrow=c(1,2))
plot(GLattice, layout=layout.fruchterman.reingold); title("5x5x5 lattice")
plot(GBlog , layout=layout.fruchterman.reingold); title("blog network")
```

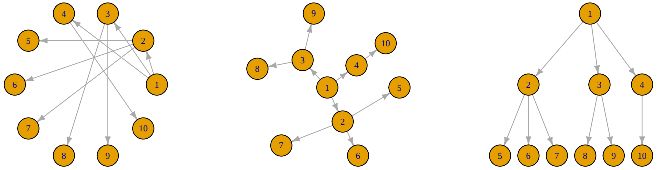




Layout and Vizualization

Do not be fooled by the plot

```r
g.tree <- graph.formula(1-+2,1-+3,1-+4,2-+5,2-+6,2-+7, 3-+8,3-+9,4-+10)
par(mfrow=c(1, 3))
igraph.options(vertex.size=30, edge.arrow.size=0.5, vertex.label=NULL)
plot(g.tree, layout=layout.circle)
plot(g.tree, layout=layout.reingold.tilford(g.tree, circular=T))
plot(g.tree, layout=layout.reingold.tilford)
```



Outline

References

- Statistical Analysis of Network Data: Methods and Models,
  Eric Kolazcyk
  Chapter 4, Sections 2 and 3
- Statistical Analysis of Network Data with R,
  Eric Kolazcyk, Gábor Csárdi
  Chapter 4, Sections 2 and 3
- Analyse statistique de graphes,
  Catherine Matias
  Chapitre 2

Outline

Vertex degree

Definition (Degree distribution)

In a graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$, recall that d_i counts the number of incident edges in $\mathcal{E}$ to i. Define f_d to be the fraction of vertices $i \in \mathcal{V}$ with degree $d_i = d$. The collection $\{f_d, d \geq 0\}$ is called the degree distribution of $\mathcal{G}$.

Property

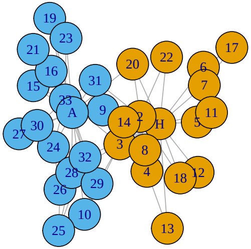
Many real world networks have a degree distribution fitting well power law distributions:

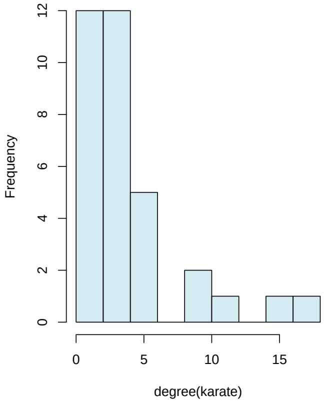
$$f_{d_i}(d) = \mathbb{P}(d_i = d) = \frac{c}{d^\gamma}, \quad c \in \mathbb{R}, \gamma > 0.$$

Those heavy-tail distributions describe few vertices with very high degrees.

Vertex degree: example I

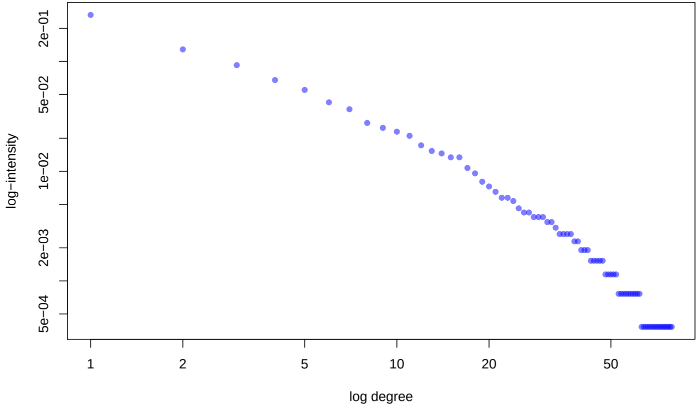
```
library(sand) data(karate)
par(mfrow=c(1,2)) plot(karate)
hist(degree(karate), col=adjustcolor("lightblue", alpha.f = 0.5), main="")
```





Vertex degree: example II

```
library(igraphdata) data(yeast)
degrees.yeast <- rev(sort(degree.distribution(yeast)))
plot(degrees.yeast[degrees.yeast!=0], log="xy", col=adjustcolor("blue", alpha.f =
0.5), pch=16, xlab="log degree", ylab="log-intensity")
```



Joint vertex degree distribution

Definition (Empirical distribution of (d_i, d_j))

Let $\mathcal{G} = (\mathcal{V}, \mathcal{E}$ be an undirected network an let $N(k, \ell)$ be the number of edges whose node have respective degrees equal to (k, ℓ) or (ℓ, k). Then the empirical distribution of (d_i, d_j) is given by

$$f_{k\ell} = \begin{cases} N(k,\ell)/2|\mathcal{E}| & \text{if } k < \ell \\ N(\ell,k)/2|\mathcal{E}| & \text{if } k > \ell \\ N(k,k)/|\mathcal{E}| & \text{if } k = \ell \end{cases}$$

Idea/principle: What kind of nodes share an edge ?

E.g. are nodes with high degrees connected with themselves or with low degree vertices?

Joint degree distribution: example for yeast PPI network

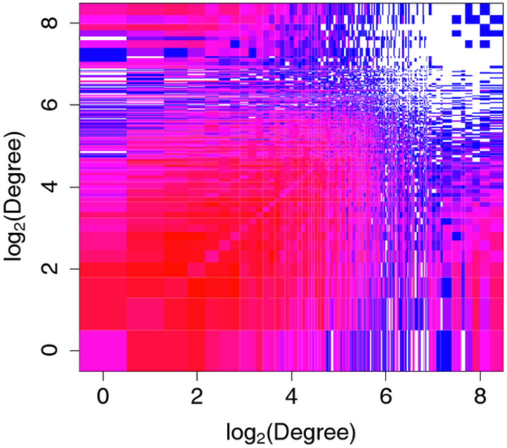


Figure: Image representation of the logarithmically transformed joint degree distribution $\log_2 f_{k\ell}$ of the yeast PPI network (*source*: E. Kolazcyk)

Distance and diameter I

Definition (distance)

- The Length of a path $e_1, \dots, e_k$ is the number of edges enterin the path (here k).
- If two nodes i, j are connected in G, then the distance ℓ_{ij} is the length of the shortest path between i and j. If the two nodes are not connected then $\ell_{ij} = \infty$.

Distance and diameter II

Definition (mean distance)

Mean distance in $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is defined by

$$\bar{\ell} = \frac{1}{n(n-1)} \sum_{(i,j)\in\mathcal{V}^2} \ell_{ij} = \frac{2}{n(n-1)} \sum_{i<j} \ell_{ij}.$$

Definition (diameter)

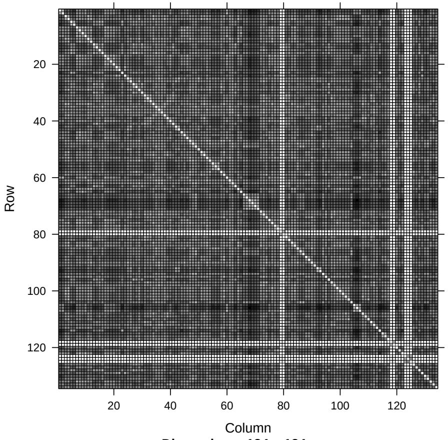
The diameter of $\mathcal{G}$ is the greatest distance between two nodes:

$$\mathrm{diameter}(\mathcal{G}) = \max_{(i,j)\in\mathcal{V}\times\mathcal{V}} (\ell_{ij})$$

Distance, Diameter: example I

```
library(Matrix)
data(ppi.CC)
diameter(ppi.CC)

## [1] 12

average.path.length(ppi.CC)

## [1] 4.448039

image(Matrix(distances(ppi.CC)))
```

Distance, Diameter: example II



Dimensions: 134 x 134

Vertex centrality: closeness

Question

How important is the node/vertice in the network?

Definition (Closeness)

Closeness is the sum of the length of the shortest paths between the node and all other nodes in the graph. It can be defined as the reciprocal of the farness:

$$C(x) = \frac{1}{\sum_y d(y,x)}.$$

$\rightsquigarrow$ *The more central a node is, the closer it is to all other nodes.*

Vertex centrality: betweenness

Question

How important is the node/vertice in the network?

Definition (Betweenness)

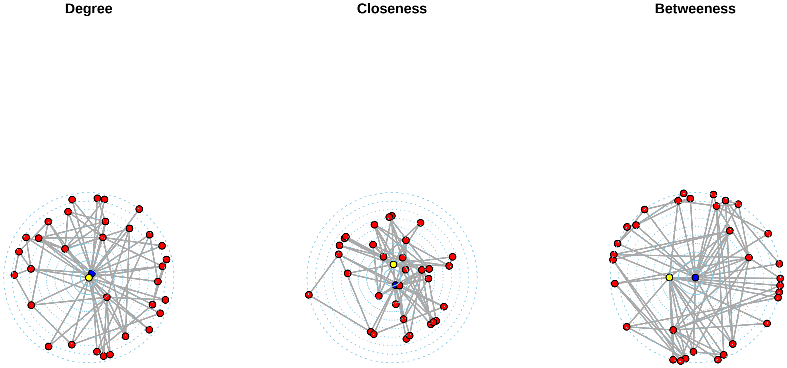
For every pairs of vertices, there exists at least one shortest path between the vertices such that the number of edges that the path passes through is minimized. The betweenness centrality for each vertex is the number of these shortest paths that pass through the vertex:

$$g(i) = \sum_{j \neq i \neq k} \frac{\sigma_{jk}(i)}{\sigma_{jk}}$$

where σ_{jk} is the total number of shortest paths from node j to node k and $\sigma_{jk}(i)$ the number of those paths that pass through i.

Example for karate club data set

administrator and instructor are in blue and yellow



Jaccard Coefficient

Definition (Jaccard Coefficient or Jaccard Index)

The Jaccard coefficient measures similarity between finite sample sets, and is defined as the size of the intersection divided by the size of the union of the sample sets:

$$J(A,B) = \frac{|A \cap B|}{|A \cup B|} = \frac{|A \cap B|}{|A| + |B| - |A \cap B|}.$$

Example

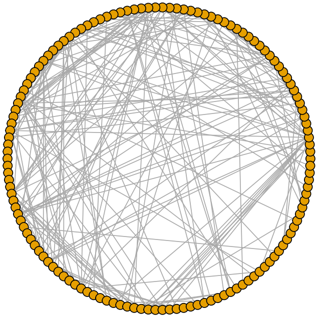
It can be used to compared two sets of egdes. For instance

- for two networks $\mathcal{G}$ and $\mathcal{H}$ defined on the same set of node, we can compare the sets $\mathcal{E}_{\mathcal{G}}$ and $\mathcal{E}_{\mathcal{H}}$.
- for a networks $\mathcal{G}$ we can compute similarity between nodes with the Jaccard index and use it to define a weighted graph of similarity.

Jaccard Coefficient: example

Plot the yeast PPI interaction network

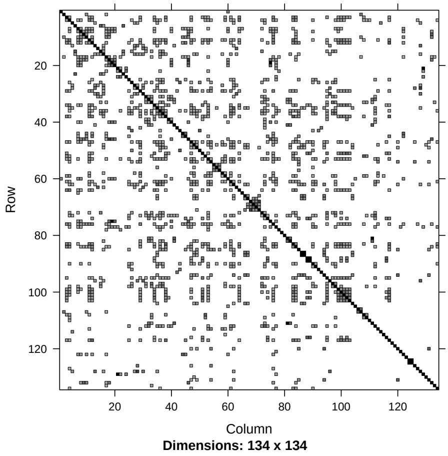
```
library(sand)
library(igraph)
plot(ppi.CC, vertex.size=6, vertex.label=NA, layout=layout_in_circle)
```



Jaccard Coefficient: example II

Compute Jaccard similarity between vertices and give a image of this

```r
library(Matrix)
image(Matrix(igraph::similarity(ppi.CC, method = "jaccard")))
```



Outline

Density

Question

Is the network locally dense in some sense?

Definition (Clique)

In an undirected graph, a clique is a subset of the vertices such that every two distinct vertices are adjacent.

Definition (Density)

The density of a (sub)-graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ is defined by

$$\mathrm{density}(\mathcal{G}) = \frac{2|\mathcal{E}|}{|\mathcal{V}|(|\mathcal{V}| - 1)} = \frac{\bar{D}}{|V| - 1},$$

where $\bar{D}$ is the mean degree of the network: how much $\mathcal{G}$ is close to a clique?

Clustering

Question

Is the network locally dense in some sense?

Definition (Triangle)

Triplets of vertices in the graph that are connected through a triangle. They correspond to transitive relationships. We let

- $\tau_\Delta(i)$ be the number of triangles in $\mathcal{G}$ where i falls.
- $\tau_3(i)$ be the number of triplets in $\mathcal{G}$ where i falls.

Definition (Clustering coefficient)

$$\mathrm{clustering}(\mathcal{G}) = \frac{1}{\mathcal{V}_2} \sum_{i \in \mathcal{V}_2} \tau_\Delta(i)/\tau_3(i),$$

where $\mathcal{V}_2$ is the set of vertices whose degree is greater or equal to 2.

Transitivity

Question

Is the network locally dense in some sense?

Definition (Triangle)

Triplet of vertices in the graph that are connected through a triangle. They correspond to transitive relationships. We let

- $\tau_\Delta(i)$ be the number of triangle in $\mathcal{G}$ where i falls.
- $\tau_3(i)$ be the number of triplet in $\mathcal{G}$ where i falls.

Definition (Transitivity)

$$\text{transitivity}(\mathcal{G}) = \frac{\sum_{\mathcal{V}} \tau_\Delta(i)}{\sum_{\mathcal{V}} \tau_3(i)},$$

Motifs

Question

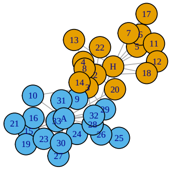
Is the network locally dense in some sense?

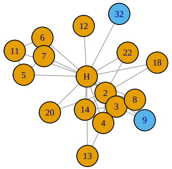
$\rightsquigarrow$ This question can be ansered thank to more complicated motifs than cliques and triangles. . .

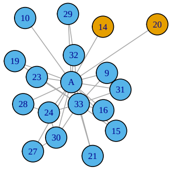
Local density: example

Create ego graphs around teacher and instructor

```
data(karate)

ego.instr <- induced.subgraph(karate, neighborhood(karate, 1, 1)[[1]])

ego.admin <- induced.subgraph(karate, neighborhood(karate, 1, 34)[[1]])
```







Local density: example II

Maximal clique size, number of triangle

```
clique.number(karate)

## [1] 5

clique.number(ego.admin)

## [1] 4

length(triangles(karate))

## [1] 135

length(triangles(ego.admin))

## [1] 51
```

Local density: example III

Efficient motif counts

```
cliques(karate, min = 5)

## [[1]]
## + 5/34 vertices, named, from 4b458a1:
## [1] Mr Hi    Actor 2  Actor 3  Actor 4  Actor 14
##
## [[2]]
## + 5/34 vertices, named, from 4b458a1:
## [1] Mr Hi   Actor 2 Actor 3 Actor 4 Actor 8

count_triangles(karate)

##  [1] 18 12 11 10  2  3  3  6  5  0  2  0  1  6  1  1  1  1  1  1  1  1  1
## [24]  4  1  1  1  1  1  4  3  3 13 15
```

Local density: example IV

Look for graph density and transitivity/clustering either globally or locally

```
graph.density(karate)

## [1] 0.1390374

graph.density(ego.instr)

## [1] 0.25

graph.density(ego.admin)

## [1] 0.2091503

transitivity(karate)

## [1] 0.2556818

transitivity(karate, "local", vids=c(1,34))

## [1] 0.1500000 0.1102941
```

Outline

References

Statistical Analysis of Network Data: Methods and Models,
Eric Kolazcyk
Chapter 4, Section 4

Statistical Analysis of Network Data with R,
Eric Kolazcyk, Gábor Csárdi
Chapter 4, Section 4

Analyse statistique de graphes,
Catherine Matias
Chapitre 3

A Tutorial on Spectral Clustering,
Ulrike von Luxburg

Principle of graph partionning

Definition (Partition)

A decomposition $\mathcal{C} = \{C_1, \dots, C_K\}$ of the vertices $\mathcal{V}$ such that

- $C_k \cap C_{k'} = \emptyset$ for any $k \neq k'$
- $\bigcup_k C_k = \mathcal{V}$

Goal of graph paritionning

Form a partition of the vertices with unsupervized approach where the $\mathcal{C}$ is composed by ''cohesive'' sets of vertices, for instance,

1. vertices well connected among themselves
2. well separated from the remaining vertices

Outline

Principle

```
Algorithm 1: Agglomerative hierarchical clustering
Input: $n$ individuals with $p$ attributes)
1 1. Compute the dissimilarity between groups
2 2. Regroup the two most similar elements
3 Iterate until all element are in a single group
Output: $n$ nested partitions from $\{\{1\},\dots,\{n\}\}$ to $\{\{1,\dots,n\}\}$
```

Ingredients

1. a dissimilarity measure between singleton
2. a distance measure between sets

Dissimilarity measures

Standards

Use standard distances on adjacency matrix:

- Euclidean distance: $x_{ij} = \sqrt{\sum_{ij} (A_{ik} - A_{jk})^2}$
- Manhattan distance: $x_{ij} = \sum_{ij} |A_{ik} - A_{jk})^2|$
- etc. . .

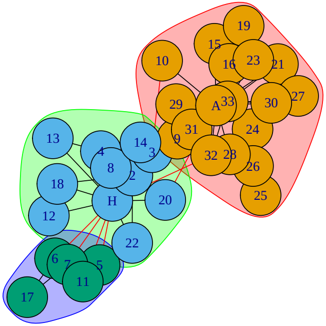
Graph-specific

For instance, Modularity (studied during tutorial)

Examples of graph clustering I

```r
hc <- cluster_fast_greedy(karate)
plot(hc,karate)
```

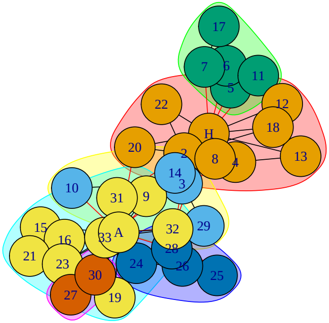
Examples of graph clustering II



Examples of graph clustering III

```r
hc <- cluster_edge_betweenness(karate)
plot(hc,karate)
```

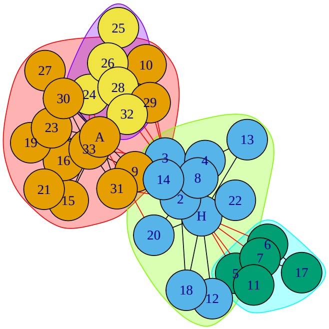
Examples of graph clustering IV



Examples of graph clustering V

```
hc <- cluster_walktrap(karate)
plot(hc,karate)
```

Examples of graph clustering VI



Outline

Graph Laplacian

Definition ((Un-normalized) Laplacian)

The Laplacian matrix $\mathbf{L}$, resulting from the modified incidence matrix $\tilde{\mathbf{B}}$ $\tilde{B}_{ij} = 1/-1$ if i is incident to j as tail/head, is defined by

$$\mathbf{L} = \tilde{\mathbf{B}}\tilde{\mathbf{B}}^\intercal = \mathbf{D} - \mathbf{A},$$

where $\mathbf{D} = \mathrm{diag}(d_i, i \in \mathcal{V})$ is the diagonal matrix of degrees.

Remark

- $\mathbf{L}$ is called Laplacian by analogy to the second order derivative (see below).
- Spectrum of $\mathbf{L}$ has much to say about the structure of the graph $\mathcal{G}$.

Graph Laplacian: spectrum

Proposition (Spectrum of $\mathbf{L}$)

The $n \times n$ matrix $\mathbf{L}$ has the following properties:

$$\mathbf{x}^\top \mathbf{L}\mathbf{x} = \frac{1}{2}\sum_{i,j} A_{ij}(x_i - x_j)^2, \quad \forall \mathbf{x} \in \mathbb{R}^n.$$

- $\mathbf{L}$ *is a symmetric, positive semi-definite matrix,*
- *the smallest eigenvalue is 0 with associated eigenvector $\mathbf{1}$.K*
- $\mathbf{L}$ *has n positive eigenvalues $0 = \lambda_1 < \cdots < \lambda_n$.*

Corollary (Spectrum and Graph)

- *The multiplicity of the first eigen value (0) of $\mathbf{L}$ determines the number of connected components in the graph.*
- *The larger the second non trivial eigenvalue, the higher the connectivity of $\mathcal{G}$.*

Normalized Graph Laplacian

Definition ((Normalized) Laplacian)

The normalized Laplacian matrix $\mathbf{L}$ is defined by

$$\mathbf{L}_N = \mathbf{D}^{-1/2}\mathbf{L}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2}.$$

Proposition

The $n \times n$ matrix $\mathbf{L}_N$ has the following properties:

$$\mathbf{x}^\top \mathbf{L}_N \mathbf{x} = \frac{1}{2}\sum_{i,j} A_{ij}\left(\frac{x_i}{\sqrt{d_i}} - \frac{x_j}{\sqrt{d_j}}\right)^2, quad \forall \mathbf{x} \in \mathbb{R}^n.$$

- $\mathbf{L}$ *is a symmetric, positive semi-definite matrix, with* n *nonnegative eigenvalues* $0 = \lambda_1 < \cdots < \lambda_n$
- *the smallest eigenvalue is* 0 *with associated eigenvector* $\mathbf{D}^{-1/2}\mathbf{1}$.

Absolute Graph Laplacian

Definition ((Absolute) Laplacian)

The absolute Laplacian matrix $\mathbf{L}_{abs}$ is defined by

$$\mathbf{L}_{abs} = \mathbf{D}^{-1/2}\mathbf{A}\mathbf{D}^{-1/2} = \mathbf{I} - \mathbf{L}_N,$$

with eigenvalues $1 - \lambda_n \leq \cdots \leq 1 - \lambda_2 \leq 1 - \lambda_1 = 1$, where $0 = \lambda_1 \leq \cdots \leq \lambda_n$ are the eigenvalues of $\mathbf{L}_N$.

Spectral Clustering

Principle

1. Use the spectral property of $\mathbf{L}$ to perform clustering in the eigen space
2. If the network have K connected components, the first K eigenvectors are $\mathbf{1}$ span the eigenspace associated with eigenvalue 0
3. Applying a simple clustering algorithm to the rows of the K first eigenvectors separate the components

$\rightsquigarrow$ This principle generalizes to a graph with a single component: spectral clustering tends to separates groups of nodes which are highly connected together

Normalized Spectral Clustering

Algorithm 2: Spectral Clustering by Ng, Jordan and Weiss (2002)

```
Input: Adjacency matrix and number of classes $Q$
1 Compute the normalized graph Laplacian $\mathbf{L}$
2 Compute the eigen vectors of $\mathbf{L}$ associated with the $Q$ smallest eigenvalues
3 Define $\mathbf{U}$, the $p \times Q$ matrix that encompasses these $Q$ vectors
4 Define $\tilde{\mathbf{U}}$, the row-wise normalized version of $\mathbf{U}$: $\tilde{u}_{ij} = \frac{u_{ij}}{\|\mathbf{U}_i\|_2}$
5 Apply k-means to $(\tilde{\mathbf{U}}_i)_{i=1,\dots,p}$
Output: vector of classes $\mathbf{C} \in \mathcal{Q}^p$, such as $C_i = q$ if $i \in q$
```

Absolute Spectral Clustering

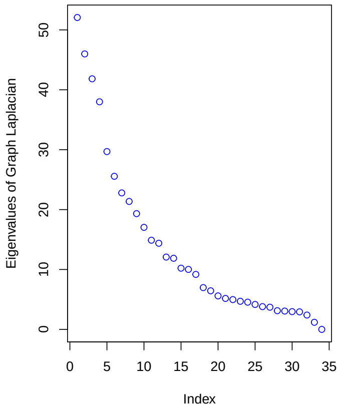
Algorithm 3: Spectral Clustering by Rohe et al. (2011)

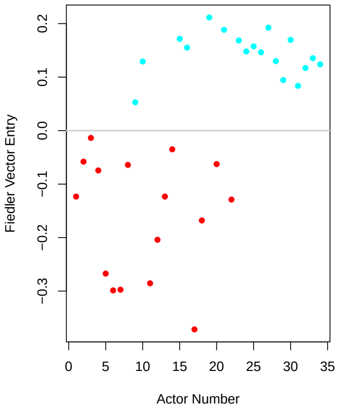
```
Input: Adjacency matrix and number of classes $Q$
1 Compute the graph Laplacian $\mathbf{L}_{abs}$
2 Compute the eigen vectors of $\mathbf{L}_{abs}$ associated with the $Q$ largest absolute
   eigenvalues
3 Define $\mathbf{U}$, the $p \times Q$ matrix that encompasses these $Q$ vectors
4 Apply k-means to $(\mathbf{U}_i)_{i=1,\dots,p}$
Output: vector of classes $\mathbf{C} \in \mathcal{Q}^p$, such as $C_i = q$ if $i \in q$
```

Example: Karate club and Fielder vector and eigenvalue I

```
k.lap <- graph.laplacian(karate)
eig.anal <- eigen(k.lap)


f.vec <- eig.anal$vectors[, 33]
faction <- get.vertex.attribute(karate, "Faction")
f.colors <- as.character(length(faction))
f.colors[faction == 1] <- "red"
f.colors[faction == 2] <- "cyan"

par(mfrow=c(1,2))
plot(eig.anal$values, col="blue",
   ylab="Eigenvalues of Graph Laplacian")
plot(f.vec, pch=16, xlab="Actor Number",
   ylab="Fiedler Vector Entry", col=f.colors)
abline(0, 0, lwd=2, col="lightgray")
```

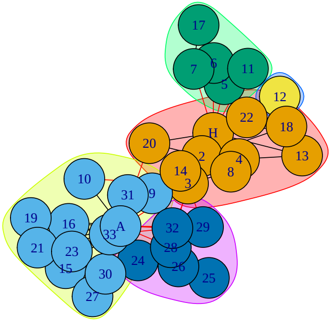
Example: Karate club and Fielder vector and eigenvalue II





Clustering based on the first non null eigenvalue

```r
hc <- cluster_leading_eigen(karate)
plot(hc,karate)
```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