02 - Network Analysis

Data Mining

SYS 6018 | Fall 2019

02-networks.pdf

Contents

1 Preliminaries

1.1 Reading

- Network Science (Chapter 2)
- MMDS 5.1-5.3, 5.5
- R package igraph

1.2 Required R Packages

We will be using the R packages of:

- igraph for network modeling
- sand for data (supplement to book *Statistical Analysis of Network Data with R* by Kolaczyk and Csárdi)
- igraphdata for some network datasets

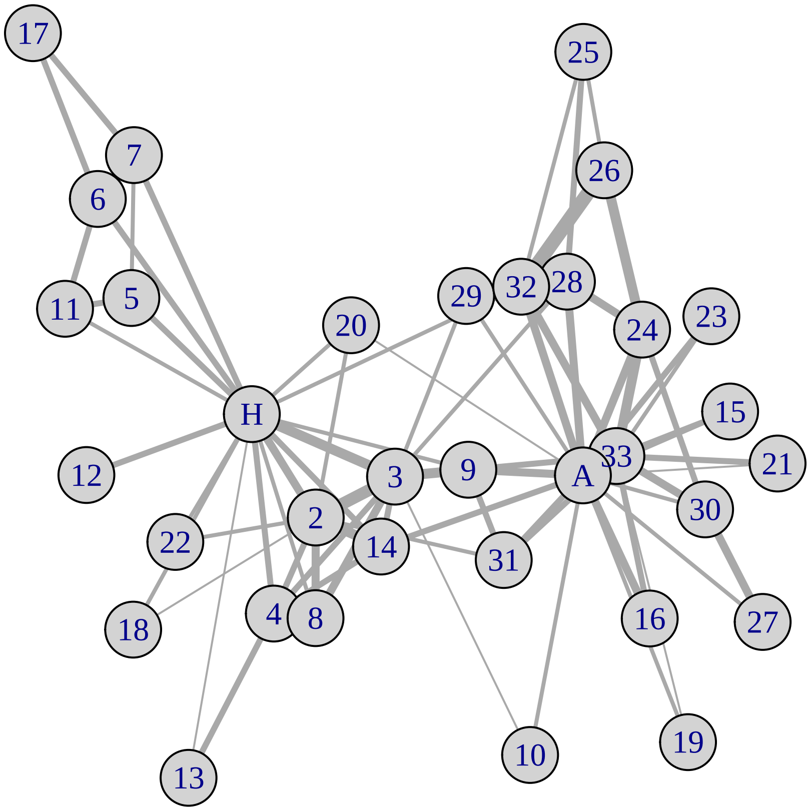
```
library(igraph)    # install.packages('igraph') if not installed
library(sand)      # install.packages('sand') if not installed
library(igraphdata)# install.packages('igraphdata') if not installed
library(tidyverse) # load last so functions are available
```

---

2 Network Intro

2.1 Example: Zachary's karate club network

```
library(igraphdata)   # for karate data
data(karate)   # type: ?karate to see description
library(igraph)
plot(karate,
     layout=layout_with_fr(karate),   # determines coordinates of nodes
     vertex.color="lightgrey",        # color of vertices
     edge.width=E(karate)$weight)     # edge weights
```



The famous karate network is based on the social network of 34 members of a university karate club. To uncover the true relationships between club members, sociologist Wayne Zachary (Wayne W. Zachary. An Information Flow Model for Conflict and Fission in Small Groups. *Journal of Anthropological Research* Vol. 33, No. 4 452-473) documented 78 pairwise links between members who regularly interacted outside the club. The edge weights represent the number of shared activities between the members.

The network experienced a singular event during the study period: a conflict between the club's president, Mr. Hi (H), and the instructor, John A (A), split the club into two; About half of the members followed the instructor and the other half the president. The breakup unveiled club's underlying community structure.

Your Turn #1 : Zachary Karate

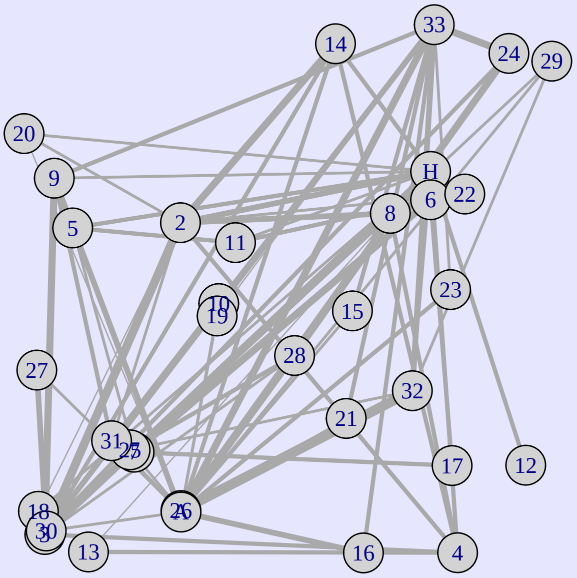
1. Do you think the graph can reveal which members will follow Mr. Hi? Why?
2. Which members will follow Mr. Hi? Why?

Solution

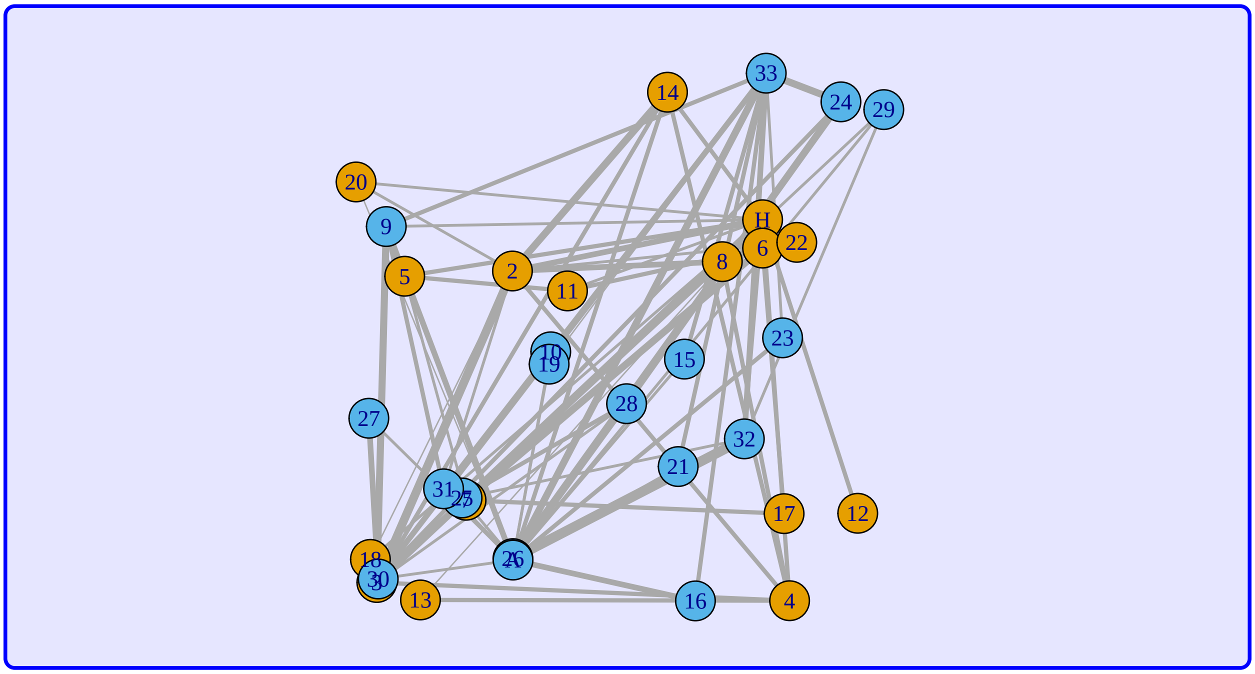
1. Yes, the members will likely choose the group that they have the best relationships with. The strength of relationship is probably associated with the edge weight.
2. Many nodes only have connections to Dr. Hi or John A.; these would be unlikely to switch allegiances. But how about the nodes with connections to both?
   - Does the graph layout (coordinates of the nodes) influence your opinion? Should it?

Community Detection is the name given to process of trying to discover the *community structure* of a network.

```
set.seed(2019)
layout.karate = layout_randomly(karate) # determines coordinates of nodes
#-- Random Layout
par(mai=c(0,0,0,0))
plot(karate,
     layout=layout.karate,            # determines coordinates of nodes
     vertex.color="lightgrey",        # color of vertices
     edge.width=E(karate)$weight)     # edge weights
```

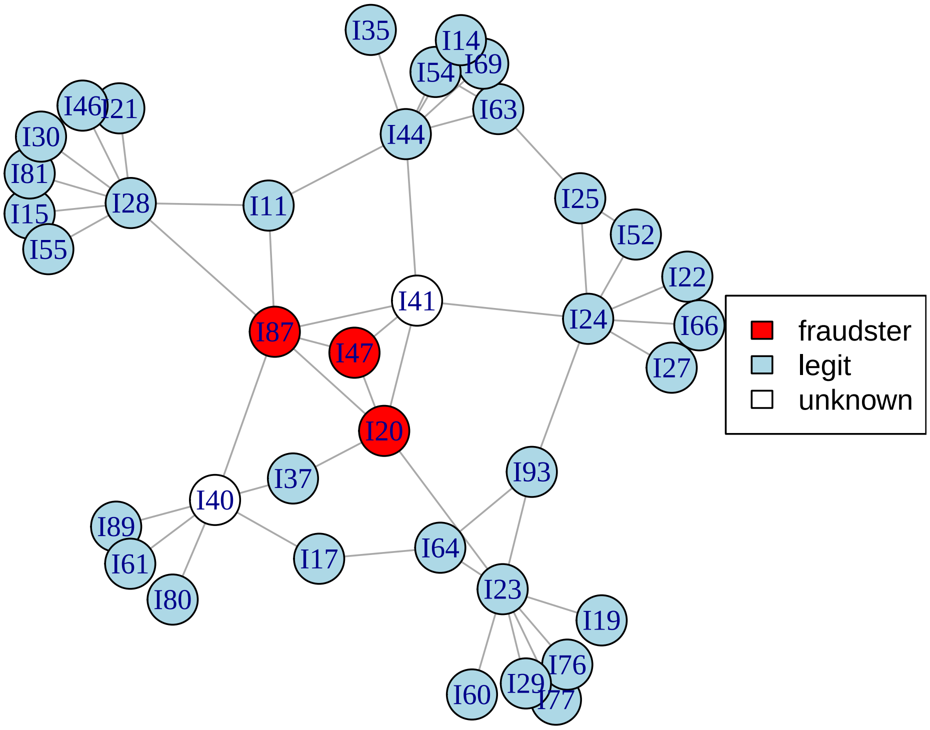


```
#-- Truth
par(mai=c(0,0,0,0))
plot(karate,
     layout=layout.karate,            # determines coordinates of nodes
     vertex.color=V(karate)$Faction,  # color of vertices by Faction
     edge.width=E(karate)$weight)     # edge weights
```



2.2 Example: Money Laundering Data

The DataCamp course Fraud Detection in R has some financial transaction data where some of the nodes (people) are engaged in fraudulence financial activities.



Your Turn #2 : Money Laundering

1. How would you classify node I40? Why?
2. How would you classify node I41? Why?
3. Does the graph layout inform your decision?

Solution

One strength of network analysis is the ability to see how nodes are connected. Is it reasonable in this network to expect that fraudsters will be connected to other fraudsters? If so, and “similar nodes are more connected to each other”, then *homophily* would suggest that the more ties to known fraudsters, the more likely you are too.

1. I40 is connected to only one fraudster directly, but how sure are we about I37, since that connects in only two hops.
2. I41 is connected to all three known fraudsters.
3. Yes, it would be much more difficult to detect in random layouts.

2.3 Community Detection for Karate

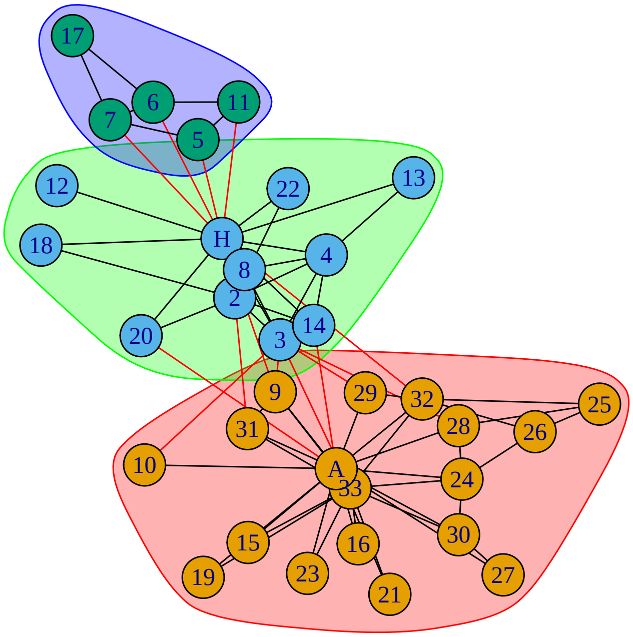
We are not going to go into details about community detection, but we can quickly run one community detection algorithm, termed *fast greedy* by igraph, that greedily optimizes something called the *modularity* score[1]. The basic idea of community detection (or network clustering) is to identify the nodes that form natural groups; usually based on the idea that nodes within the same community should have a higher probability of being connected to each other than to members of other communities.

Santo Fortunato is a good place to start if you are interested in learning more:

- Community detection in networks: A user guide https://arxiv.org/abs/1608.00163
- Community detection in graphs https://arxiv.org/abs/0906.0612

```
#-- Run community detection
fg = cluster_fast_greedy(karate)
membership(fg)
#>    Mr Hi  Actor 2  Actor 3  Actor 4  Actor 5  Actor 6  Actor 7  Actor 8
#>        2        2        2        2        3        3        3        2
#>  Actor 9 Actor 10 Actor 11 Actor 12 Actor 13 Actor 14 Actor 15 Actor 16
#>        1        1        3        2        2        2        1        1
#> Actor 17 Actor 18 Actor 19 Actor 20 Actor 21 Actor 22 Actor 23 Actor 24
#>        3        2        1        2        1        2        1        1
#> Actor 25 Actor 26 Actor 27 Actor 28 Actor 29 Actor 30 Actor 31 Actor 32
#>        1        1        1        1        1        1        1        1
#> Actor 33   John A
#>        1        1

#-- igraph has a built in plotting for communities
plot(fg, karate)
```

[1] A Clauset, MEJ Newman, C Moore: Finding community structure in very large networks



The fast-greedy community detection algorithm suggests there are 3 communities: one involving H, one A, and another that is connected to H, but tends to be more connected to each other than other nodes in H's community.

Community detection is equivalent to clustering the nodes of a network. Like we will see later in the course (Clustering Section), there is no one best way to cluster. As with most unsupervised methods, community detection is best thought of as an exploratory, rather than confirmatory, approach.

3 Basic Network Concepts

3.1 Basic Definitions

- A graph can be represented by $G = (V, E)$ where V are the set of vertices (also called nodes) and E is a set of edges (also called links).
- There are $|V|$ nodes and $|E|$ edges in G
- The edge set E is a collection of pairs, (u, v) where $u, v \in V$
  - For undirected graphs, (u, v) is same as (v, u).
  - For directed graphs (digraph), (u, v) is distinct from (v, u)

3.2 Creating a Network

- A network needs two components:
  1. Nodes
  2. Edges
- **Nodes**: data frame of node labels and (optional) node attributes

```
nodes = tibble(node=1:7, group=c(1,1,2,2,1,2,1))
#> # A tibble: 7 x 2
#>    node group
#>   <int> <dbl>
#> 1     1     1
#> 2     2     1
#> 3     3     2
#> 4     4     2
#> 5     5     1
#> 6     6     2
#> 7     7     1
```

- **Edges**: data frame of edges
  - Common to use labels *from* and *to*, even for *undirected* networks
  - optional edge attributes

```
edges = tibble(from = c(1,1,2,2,3,4,4,6,4,5,6,6),
               to =   c(2,3,3,4,5,5,6,4,7,6,5,7),
               weight = c(1,1,2,2,3,3,2,2,1,1,2,2)) # edge weight
edges
#> # A tibble: 12 x 3
#>     from    to weight
#>    <dbl> <dbl>  <dbl>
#>  1     1     2      1
#>  2     1     3      1
#>  3     2     3      2
#>  4     2     4      2
#>  5     3     5      3
#>  6     4     5      3
#>  7     4     6      2
#>  8     6     4      2
#>  9     4     7      1
#> 10     5     6      1
#> 11     6     5      2
#> 12     6     7      2
```

- R igraph package
  - The igraph package is one package in R to help with network data

```
library(igraph)
#-- Undirected Graph
g = graph_from_data_frame(d=edges, vertices=nodes, directed=FALSE)
g
#> IGRAPH 66be006 UNW- 7 12 --
#> + attr: name (v/c), group (v/n), weight (e/n)
#> + edges from 66be006 (vertex names):
#>  [1] 1--2 1--3 2--3 2--4 3--5 4--5 4--6 4--6 4--7 5--6 5--6 6--7

#-- Directed Graph
g_dir = graph_from_data_frame(d=edges, vertices=nodes, directed=TRUE)
g_dir
#> IGRAPH 66bec33 DNW- 7 12 --
#> + attr: name (v/c), group (v/n), weight (e/n)
#> + edges from 66bec33 (vertex names):
#>  [1] 1->2 1->3 2->3 2->4 3->5 4->5 4->6 6->4 4->7 5->6 6->5 6->7
```

- Node information is stored in the object `V(g)`

```
vertex_attr(g)    # get all node attributes
#> $name
#> [1] "1" "2" "3" "4" "5" "6" "7"
#>
#> $group
#> [1] 1 1 2 2 1 2 1

V(g)$name  # get vector of the names
#> [1] "1" "2" "3" "4" "5" "6" "7"

V(g)$group # get vector of group info
#> [1] 1 1 2 2 1 2 1
```

- Edge information is stored in the object `E(g)`

```
edge_attr(g)    # get all node attributes
#> $weight
#>  [1] 1 1 2 2 3 3 2 2 1 1 2 2

E(g)$weight  # get vector of weights
#>  [1] 1 1 2 2 3 3 2 2 1 1 2 2

tibble(edge = attr(E(g), "vnames"),  # make into a dataframe
       weight = E(g)$weight)
#> # A tibble: 12 x 2
#>    edge  weight
#>    <chr>  <dbl>
#>  1 1|2        1
#>  2 1|3        1
#>  3 2|3        2
#>  4 2|4        2
#>  5 3|5        3
#>  6 4|5        3
#>  7 4|6        2
#>  8 4|6        2
#>  9 4|7        1
#> 10 5|6        1
#> 11 5|6        2
#> 12 6|7        2
```

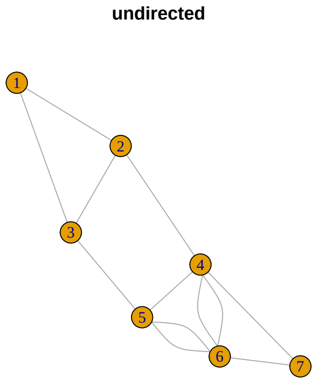
3.3 Visualizing a Network

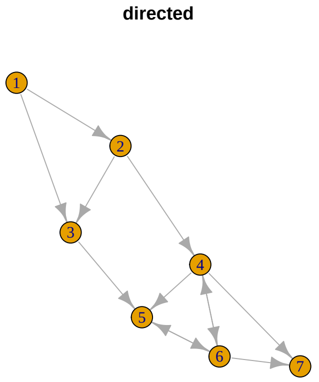
3.3.1 Graph Layout

Graph layouts are projections of the vertices and edges into some space. Different layouts reveal different aspects of a graph.

- Note: 2D layouts can be very misleading; don't trust your eyes
- Choose the layout to help reveal the structure. In `igraph`,
  - `layout.fructerman.reingold` is a spring-embedder method
  - `layout.kamada.kawai` is based on multidimensional scaling (MDS)
  - These will be a function of the *distance* between vertices

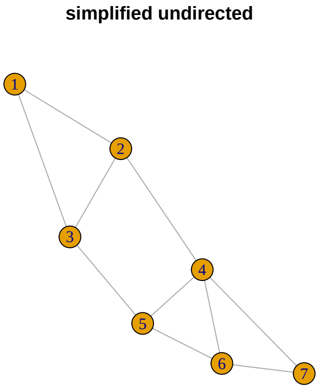
```
g.layout = layout_with_fr(g) # create layout (node coordinates)
plot(g, layout=g.layout, main="undirected")      # plot undirected graph
plot(g_dir, layout=g.layout, main="directed")    # plot directed graph
```





- Notice that we have multiple edges in the *undirected* graph. We can simplify the graph into a *proper* undirected graph (with only a single edge between nodes).

```
# Note: there is a conflict with purrr::simplify() and igraph::simplify(),
#  thus I will be specific that I want igraph's simplify function.
g = igraph::simplify(g)     # this removes multiple edges, loops, and combines edge
plot(g, layout=g.layout, main="simplified undirected")      # plot undirected graph
```



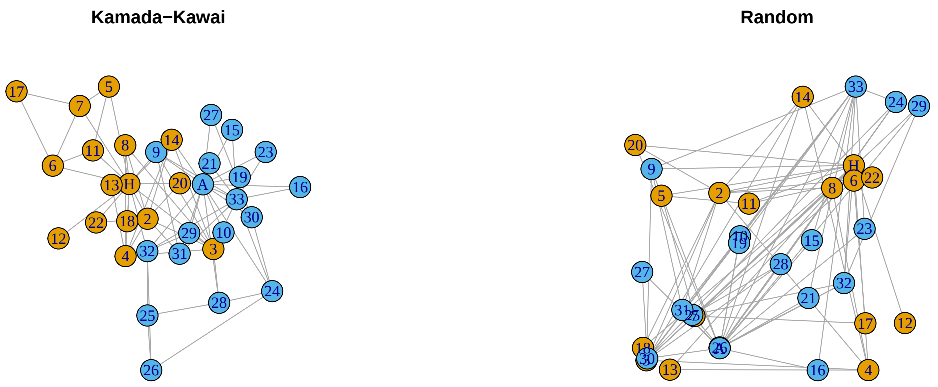
Don't miss the important information in the code comments about `igraph::simplify()`:

- if the argument `remove.multiple=TRUE` (the default setting), then all edge attributes are combined (e.g., summed).
- The graph now has single edges only, and the weights are aggregated.

```
#- Notice the difference from the previous version
tibble(edge = attr(E(g), "vnames"),
       weight = E(g)$weight)
#> # A tibble: 10 x 2
#>    edge  weight
#>    <chr>  <dbl>
#>  1 1|2        1
#>  2 1|3        1
#>  3 2|3        2
#>  4 2|4        2
#>  5 3|5        3
#>  6 4|5        3
#>  7 4|6        4
#>  8 4|7        1
#>  9 5|6        3
#> 10 6|7        2
```

- The layout can have a **big** influence on how you perceive the network

```
plot(karate, layout=layout_with_kk(karate), main="Kamada-Kawai")  # Kamada-Kawai la
plot(karate, layout=layout_randomly(karate), main="Random")       # Random layout
```

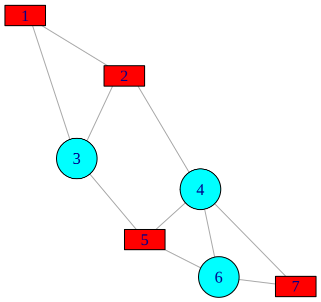

Kamada−Kawai

Random

3.3.2 Graph Decoration

- The nodes and edges can be *decorated* with color, size, shape, etc.

```
plot(g, layout=g.layout,
   vertex.size=30,
   vertex.shape=ifelse(V(g)$group==1, "rectangle", "circle"),
   vertex.color=ifelse(V(g)$group==1, "red", "cyan"))
```



3.4 Representations for Graphs

3.4.1 Edge List

An edge list is usually represented as a two-column matrix (or data.frame)

```
get.edgelist(g)
#>       [,1] [,2]
#>  [1,] "1"  "2"
#>  [2,] "1"  "3"
#>  [3,] "2"  "3"
#>  [4,] "2"  "4"
#>  [5,] "3"  "5"
#>  [6,] "4"  "5"
#>  [7,] "4"  "6"
#>  [8,] "4"  "7"
#>  [9,] "5"  "6"
#> [10,] "6"  "7"
```

3.4.2 Adjacency Matrix

An adjacency matrix is the $|V| \times |V|$ matrix, $\mathbf{A}$ such that

$$A_{ij} = \begin{cases} 1, & \text{if } \{i, j\} \in E, \\ 0, & \text{otherwise} \end{cases}$$

For undirected graphs, the adjacency matrix will by symmetric.

```
get.adjacency(g)     # binary and symmetric
#> 7 x 7 sparse Matrix of class "dgCMatrix"
#>   1 2 3 4 5 6 7
#> 1 . 1 1 . . . .
#> 2 1 . 1 1 . . .
#> 3 1 1 . . 1 . .
#> 4 . 1 . . 1 1 1
#> 5 . . 1 1 . 1 .
#> 6 . . . 1 1 . 1
#> 7 . . . 1 . 1 .
get.adjacency(g_dir)     # binary and not-symmetric
#> 7 x 7 sparse Matrix of class "dgCMatrix"
#>   1 2 3 4 5 6 7
#> 1 . 1 1 . . . .
#> 2 . . 1 1 . . .
#> 3 . . . . 1 . .
#> 4 . . . . 1 1 1
#> 5 . . . . . 1 .
#> 6 . . . 1 1 . 1
#> 7 . . . . . . .
```

3.4.3 Adjacency List

The adjacency list is an array (in R, a list) of size $|V|$, where the elements of the list indicate the set of vertices that are adjacent. It is essentially the sparse representation of the adjacency matrix.

```
get.adjlist(g)
#> $`1`
#> + 2/7 vertices, named, from 66d7437:
#> [1] 2 3
#>
#> $`2`
#> + 3/7 vertices, named, from 66d7437:
#> [1] 1 3 4
#>
#> $`3`
#> + 3/7 vertices, named, from 66d7437:
#> [1] 1 2 5
#>
#> $`4`
#> + 4/7 vertices, named, from 66d7437:
#> [1] 2 5 6 7
#>
#> $`5`
#> + 3/7 vertices, named, from 66d7437:
#> [1] 3 4 6
#>
#> $`6`
#> + 3/7 vertices, named, from 66d7437:
#> [1] 4 5 7
#>
#> $`7`
#> + 2/7 vertices, named, from 66d7437:
#> [1] 4 6
```

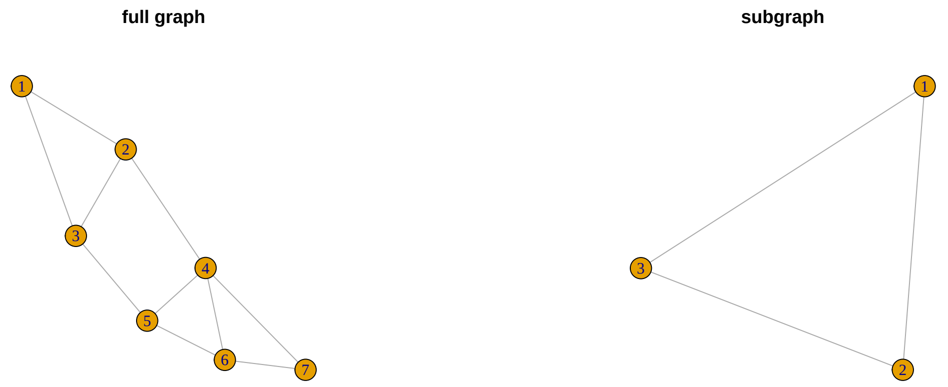
3.5 Weighted Edges

- Edges can have attributes that describe the nature of the connection between two vertices
- An example is to assign edge weights $\{w_{ij} : e_{ij} \in E\}$
  - Weights can be measurements of things like: flow rate, number of transactions, call time, travel speed, etc.
- More generally, consider the weight matrix W, which is the $|V| \times |V|$ matrix containing the edge weights. The weights will be $W_{ij} = 0$ if $A_{ij} = 0$.
  - The adjacency matrix is a special case of weight matrix with binary weights

3.6 Subgraphs

- A graph $H = (V_H, E_H)$ is a subgraph of $G = (V_G, E_G)$ if $V_H \subseteq V_G$ and $E_H \subseteq E_G$.
- An *induced subgraph* of graph G is a subgraph $G' = (V', E')$ where $V' \subseteq V$ is a pre-specified subset of vertices and $E' \subseteq E$ is the collection of edges to be found in G among that subset of vertices.

```
g3 = induced_subgraph(g, v=1:3)    # only select vertices 1:3
plot(g, layout=g.layout, main='full graph')
plot(g3, main='subgraph')
```



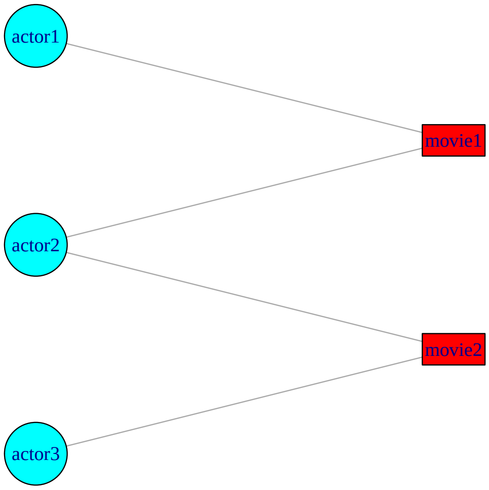
full graph

subgraph

3.7 Bipartite graphs

A bipartite graph (also called *two-mode*) is a graph $G = (V, E)$ such that the vertex set V may be partitioned into two disjoint sets V_1 and V_2, and each edge in E has one endpoint in V_1 and the other in V_2.

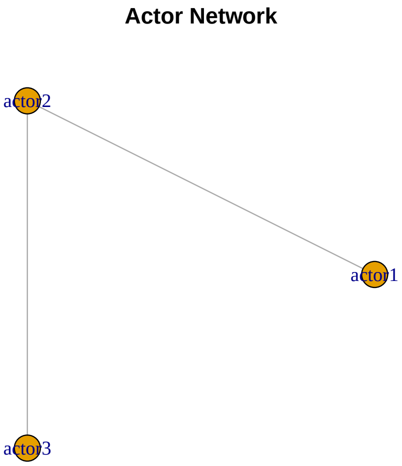
```
g.bip <- graph.formula(actor1:actor2:actor3,
   movie1:movie2, actor1:actor2 - movie1,
   actor2:actor3 - movie2)
V(g.bip)$type <- grepl("^movie", V(g.bip)$name)
plot(g.bip, layout=-layout.bipartite(g.bip)[,2:1],
   vertex.size=30, vertex.shape=ifelse(V(g.bip)$type,
     "rectangle", "circle"),
   vertex.color=ifelse(V(g.bip)$type, "red", "cyan"))

get.incidence(g.bip)          # get the incidence matrix
#>         movie1 movie2
#> actor1       1      0
#> actor2       1       1
#> actor3       0       1
```



Some examples:
- Membership networks: V_1 are the members and V_2 the organizations
- Recommender data: V_1 are the movies and V_2 the reviewers
- Market basket data: V_1 are the shoppers and V_2 are the items in the store
- Travel: V_1 are the people and V_2 are the places they visit

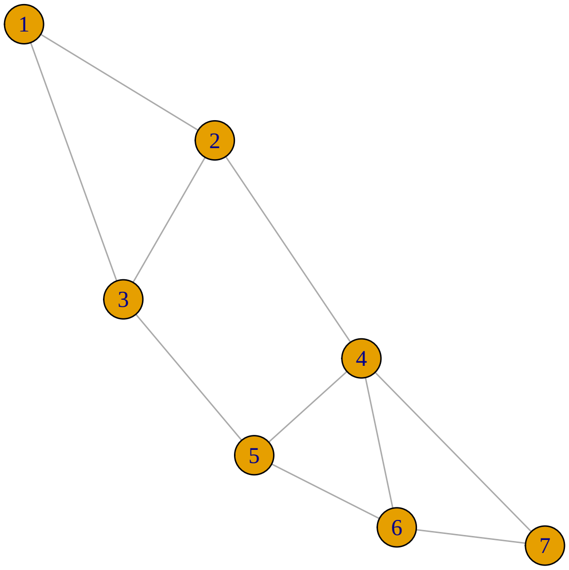
A bipartite graph can be accompanied by the induced subgraph formed by connecting the vertices, say V_1, by assigning an edge to vertices that edges in E to at least one common vertex in V_2

```
plot(bipartite.projection(g.bip)$proj1,main="Actor Network",
     layout=layout_in_circle)
```



3.8 Graphs and Matrix Notation

We will be using our example graph



3.8.1 Adjacency matrix

$$A_{ij} = \begin{cases} 1, & \text{if } \{i, j\} \in E, \\ 0, & \text{otherwise} \end{cases}$$

3.8.2 Degree

- The row sums give the vertex *degree*,

  $$d_i = \sum_j A_{ij}$$

  which is the number of edges vertex i is connected to

```
A = get.adjacency(g, sparse=FALSE)
A
#>   1 2 3 4 5 6 7
#> 1 0 1 1 0 0 0 0
#> 2 1 0 1 1 0 0 0
#> 3 1 1 0 0 1 0 0
#> 4 0 1 0 0 1 1 1
#> 5 0 0 1 1 0 1 0
#> 6 0 0 0 1 1 0 1
#> 7 0 0 0 1 0 1 0
rowSums(A)           # degree from adjacency matrix
#> 1 2 3 4 5 6 7
#> 2 3 3 4 3 3 2
degree(g)            # using igraph::degree() function
#> 1 2 3 4 5 6 7
#> 2 3 3 4 3 3 2
```

- For directed graphs (digraphs), $d_i^{out} = \sum_j A_{ij}$ and $d_i^{in} = \sum_j A_{ji}$
  - rowsums or colsums

```
A2 = get.adjacency(g_dir, sparse=FALSE)
A2
#>   1 2 3 4 5 6 7
#> 1 0 1 1 0 0 0 0
#> 2 0 0 1 1 0 0 0
#> 3 0 0 0 0 1 0 0
#> 4 0 0 0 0 1 1 1
#> 5 0 0 0 0 0 1 0
#> 6 0 0 0 1 1 0 1
#> 7 0 0 0 0 0 0 0
degree(g_dir, mode="in")   # colSums(A2)
#> 1 2 3 4 5 6 7
#> 0 1 2 2 3 2 2
degree(g_dir, mode="out")  # rowSums(A2)
#> 1 2 3 4 5 6 7
#> 2 2 1 3 1 3 0
```

- For weighted graphs, the graph *strength* is the respective sums of the weight matrix W. See `igraph::strength()`

3.8.3 Movement on a graph

- A *walk* on a graph G describes a sequence of adjacent vertices $(v_0, v_1, ..., v_n)$, where each v_i is connected to v_{i+1} by an edge.
- A *connected* graph is one where a walk exists between every pair of vertices
- *Geodesic distance* (also called *number of hops*) is the length of the shortest path between two vertices

```
distances(g, weights=NA)    # geodesic or shortest-path distances
#>   1 2 3 4 5 6 7
#> 1 0 1 1 2 2 3 3
#> 2 1 0 1 1 2 2 2
#> 3 1 1 0 2 1 2 3
#> 4 2 1 2 0 1 1 1
#> 5 2 2 1 1 0 1 2
#> 6 3 2 2 1 1 0 1
#> 7 3 2 3 1 2 1 0

distances(g, weights=E(g)$weight)   # use edge weights
#>   1 2 3 4 5 6 7
#> 1 0 1 1 3 4 6 4
#> 2 1 0 2 2 5 5 3
#> 3 1 2 0 4 3 6 5
#> 4 3 2 4 0 3 3 1
#> 5 4 5 3 3 0 3 4
#> 6 6 5 6 3 3 0 2
#> 7 4 3 5 1 4 2 0
```

- The matrix power, A^r gives the number of walks of length r between vertices

```
#- set r
r = 2     # walks of length 2

#- Direct method
Ar = diag(nrow(A))
for(i in 1:r) {Ar <- Ar %*% A}    # r = 2
Ar
#>       1 2 3 4 5 6 7
#> [1,] 2 1 1 1 1 0 0
#> [2,] 1 3 1 0 2 1 1
#> [3,] 1 1 3 2 0 1 0
#> [4,] 1 0 2 4 1 2 1
#> [5,] 1 2 0 1 3 1 2
#> [6,] 0 1 1 2 1 3 1
#> [7,] 0 1 0 1 2 1 2

#- eigen method
eig = eigen(A)
Ar2 = eig$vectors %*% diag(eig$values^r) %*% solve(eig$vectors)
round(Ar2)
#>      [,1] [,2] [,3] [,4] [,5] [,6] [,7]
#> [1,]    2    1    1    1    1    0    0
#> [2,]    1    3    1    0    2    1    1
#> [3,]    1    1    3    2    0    1    0
#> [4,]    1    0    2    4    1    2    1
#> [5,]    1    2    0    1    3    1    2
#> [6,]    0    1    1    2    1    3    1
#> [7,]    0    1    0    1    2    1    2
```

Let A be an $n \times n$ matrix with eigen-decomposition:

$$\begin{aligned} Ax &= \lambda x \\ AAx &= A\lambda x \qquad \text{multiple both sides by } A \\ &= \lambda^2 x \qquad \text{because } Ax = \lambda x \end{aligned}$$

Let $A = V\Lambda V^{-1}$ where Λ is a diagonal matrix of eigenvalues and V the orthogonal matrix of eigenvectors.

$$\begin{aligned} AA &= (V\Lambda V^{-1})(V\Lambda V^{-1}) \\ &= V\Lambda^2 V^{-1} \end{aligned}$$

And thus,

$$\begin{aligned} A(AA) &= (V\Lambda V^{-1})V\Lambda^2 V^{-1} \\ &= V\Lambda^3 V^{-1} \end{aligned}$$

and so on.

- *Graph Laplacian* is the $|V| \times |V|$ matrix $L = D - A$, where $D = \text{diag}[d_i : i \in V]$ is the diagonal matrix with degree along the diagonal. It is useful for calculating:

$$\mathbf{x}^{\mathsf{T}} L \mathbf{x} = \sum_{\{i,j\} \in E} (x_i - x_j)^2$$

  for $\mathbf{x} \in \mathbb{R}^{|V|}$.

4 Homophily, Assortativity, and Fraud Prediction

4.1 Homophily

> "Birds of a feather flock together"
>
> "Misery loves company"

McPherson et al (2001)[2] observed that people's personal/social networks are homogeneous with regard to many sociodemographic, behavioral, and intrapersonal characteristics. As such, contact contact between similar people occur at a higher rate than among dissimilar people; this principal is termed *homophily* (greek: same + love/affection).

Perhaps the most basic source of homophily is **space**:

> *We are more likely to have contact with those who are closer to us in geographic location than those who are distant.*

Zipf (1949) stated the principle as a matter of effort: It takes more energy to connect to those who are far away than those who are readily available.

4.1.1 Examples:

- **Political Blogs:**[3]

[2] McPherson, M., Smith-Lovin, L., & Cook, J. M. (2001). Birds of a Feather: Homophily in Social Networks. *Annual Review of Sociology*, 27, 415–444

[3] Lada A. Adamic and Natalie Glance. 2005. The political blogosphere and the 2004 U.S. election: divided they blog. In Proceedings of the 3rd international workshop on Link discovery (LinkKDD '05). ACM, New York, NY, USA

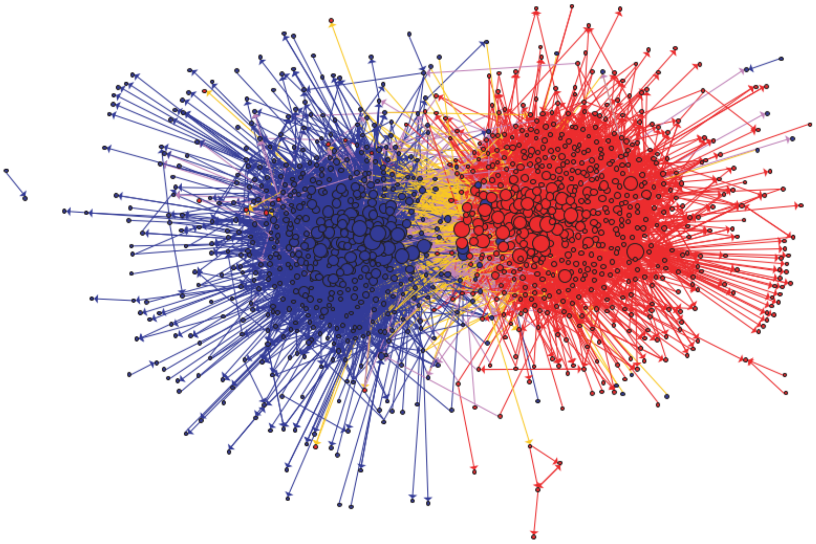
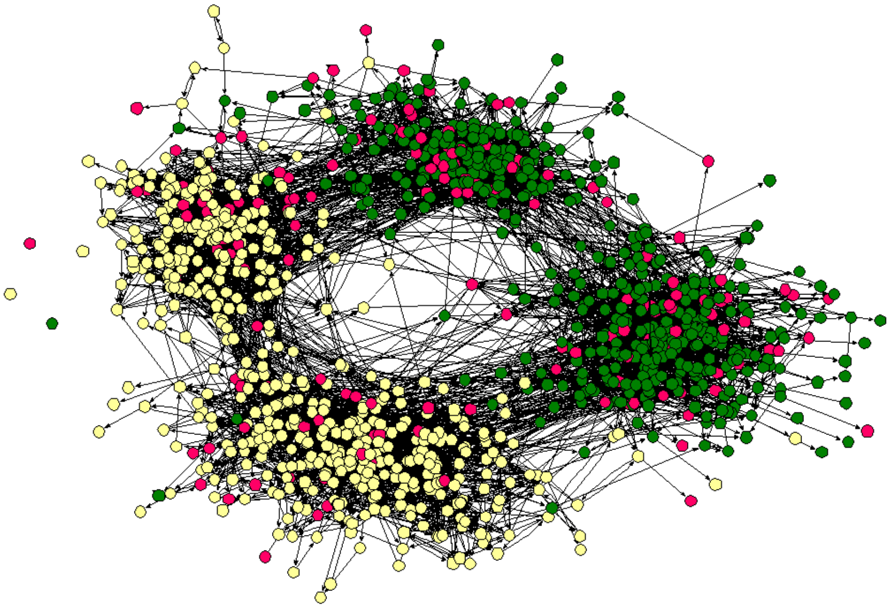


Figure 1: Community structure of political blogs (expanded set), shown using utilizing a GEM layout [11] in the GUESS[3] visualization and analysis tool. The colors reflect political orientation, red for conservative, and blue for liberal. Orange links go from liberal to conservative, and purple ones from conservative to liberal. The size of each blog reflects the number of other blogs that link to it.

- **School Segregation:**[4]

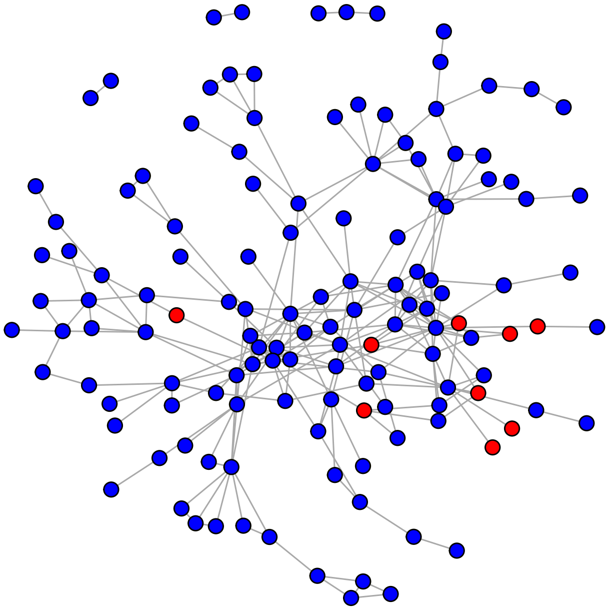


Nodes are students in a high school and two nodes are connected if one student named the other student as friend (the data was collected as part of the Add Health study). The color of the nodes corresponds to the race of the students. As we can see, "yellow" students are much more likely to be friends with other yellow students and "green" students are more likely to connect to other green students. (Interestingly, the "pink" students, who

[4] Moody (2001) "Race, school integration, and friendship segregation in America," *American Journal of Sociology* 107, 679-716. Figure taken from: http://networksciencebook.com/chapter/7#summary7. Text taken from: http://social-dynamics.org/homophily/

are in the vast minority seem to be distributed throughout the network.

- **Yeast protein interaction network**[5] *Notice that the red nodes are not connected to other red nodes.*



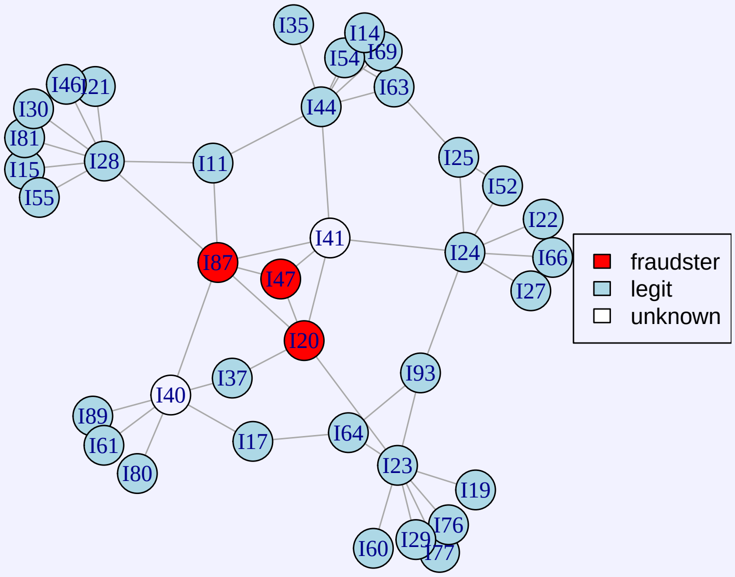
4.2 Node Prediction

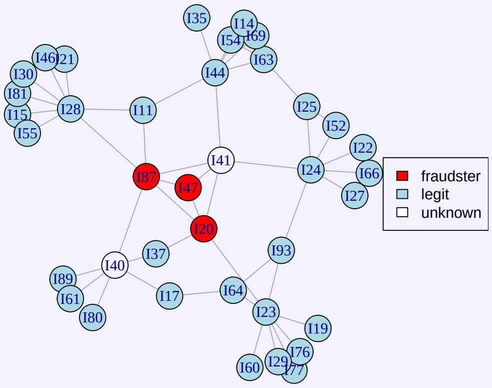
- If there is homophily in the network, then we can expect **nodes with similar attributes to be connected by an edge**.
- More specifically, under homophily, we might expect that node attributes could be predicted from the attributes of its closest neighbors.

Your Turn #3

Consider the *Money Laundering* network.

[5] X. Jiang, N. Nariai, M. Steffen, S. Kasif, E. Kolaczyk (2008) "Integration of relational and hierarchical network information for protein function prediction". *BMC Bioinform.* 9, 350. https://www.ncbi.nlm.nih.gov/pmc/articles/PMC2535605/. Data accessed from the R`sand` package: `data(ppi.CC, package="sand")`. Color indicates whether the protein contains the 'rho GTPase-activating protein domain' (IPR000198) motif.





1. Write an algorithm to *estimate the probability* that an unlabeled node is a fraudster.
2. What should your algorithm predict for nodes I40 and I41?
3. What if the node has no neighbors (i.e., degree of 0)?
4. How would you assess the *uncertainty* in your estimate?
5. How would your approach change if the network had weights or directed edges?

Solution

- Let $x_i \in \{0, 1\}$ be the fraud label (node attribute) of node i, where $x_i = 1$ means node i is a fraudster and $x_i = 0$ means they are not a fraudster.
- Let $\Gamma(i) = \{j : A_{ij} = 1 \text{ or } A_{ji} = 1\}$ be the *ego neighborhood* of i. This is the set of nodes connected to node i in one hop.
- Let $d_i = \sum_j A_{ij}$ be the **degree** of node i for undirected and unweighted graphs. (Use `igraph::strength()` for weighted degree.)

1. Algorithm to estimate the probability that node i is a fraudster.
   a. Find all neighbors of node i, $\Gamma(i)$.
   b. Get the label for all neighbors, $\mathcal{X} = \{x_j : j \in \Gamma(i)\}$.

c. Estimate the probability as $\hat{p} = \frac{\sum_{j \in \Gamma(i)} x_i}{|\Gamma(i)|}$.

2. $\hat{p}(I40) = 1/6$ and $\hat{p}(I41) = 3/5$. So would go with I41 as fraud and I40 as not fraud if I had to make a hard classification.
3. What if the node has no neighbors (i.e., degree of 0)?

Let p_0 be a prior (*apriori*) probability that any node is a fraudster. Then any node with no edges would get this probability.

4. Uncertainty.

There are a couple ways to think about uncertainty.

i. If we knew p, then there is uncertainty in whether the node is fraud or not. I.e., p close to 0 or 1 has less uncertainty than $p = .5$.

ii. We are less certain *of our estimate* when its degree is smaller. Think standard error $SE(p) = \sqrt{\hat{p}(1-\hat{p})/n}$ where $n = d_i$. So its a function of $1/\sqrt{d_i}$ (**if there is independence**, which we can not reasonably say).

Think of it this way: if we only have one observation to predict from, then we should have more uncertainty than if the edge is connected to 10 other nodes?

- One way to account for this is to use a weighted estimate.
  - Make the estimate somewhere between the observed $\hat{p} = n/N$ and prior p_0.
  - The larger the neighborhood, the closer to $\hat{p}$.
  - $\hat{p}\pi_i + (1 - \pi_i)p_0$ where $0 \leq \pi_i \leq 1$ is the weight for node i.
- Use $\pi_i = d_i/(d_i + k)$, where k is the shrinkage factor and d_i is the degree (neighborhood size).
- This is equivalent to a concept called *Laplace Smoothing*. Think about adding k additional *pseudo* nodes with $x_j = p_0$ which all have an edge connecting to node i.
  - Now, there are k more nodes in the neighborhood, each contributing p_0 (instead of a $\{0, 1\}$).
  - The new estimate is

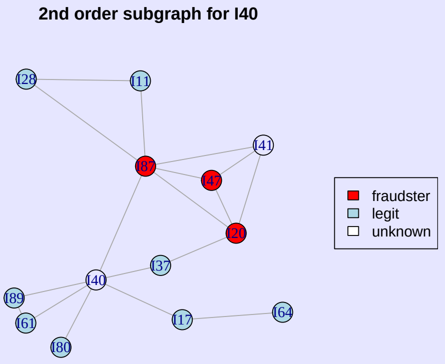
$$\frac{\left(\sum_{j \in \Gamma(i)} x_i\right) + kp_0}{|\Gamma(i)| + k}$$

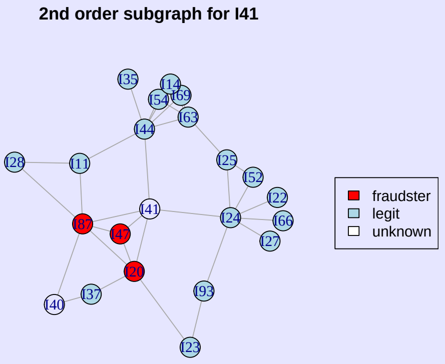
- More generally, let x_i be probability of fraudster.

iii) The other type of uncertainty (variance in bias/variance trade-off) is in sensitivity to the network structure and which nodes are missing. See next section for evaluation.

5. Extensions

- Weighted edges
- directed edges
- ego-centric neighborhood





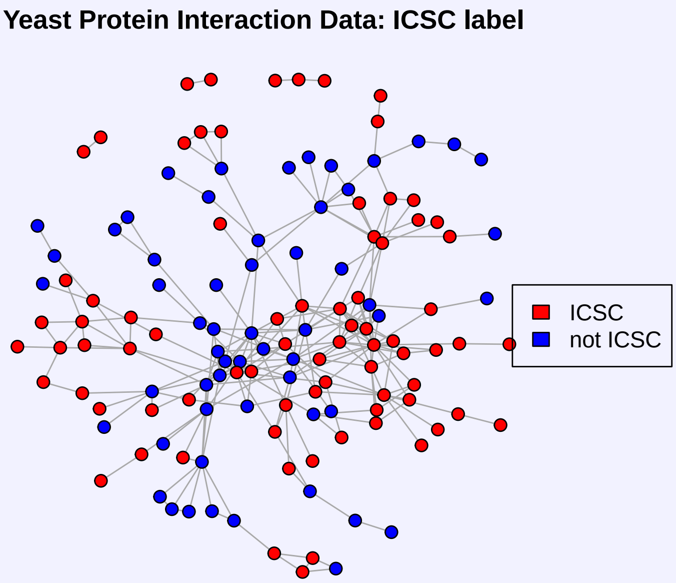
4.2.1 Testing the Node Prediction Algorithm

We can use a type of *resampling* to evaluate how well our algorithm might do on an actual network.

1. Take a real network with binary/categorical label
2. Randomly remove some node labels (for some fraction f)
3. Run the algorithm (using different values of k)
4. Record results
5. Evaluate effects of f and k.

Your Turn #4

Evaluate how well the simple nearest neighbor method works on the Yeast Protein Interaction Data for predicting the `ICSC` attribute which indicates whether the protein is annotated with the "intracellular signaling cascade" GO term. It takes a binary (zero or one) value.



Examine the results for different values of f and k. See the R code `node-predict.R` from the course website for help.

4.3 Link Prediction

It can also be useful to have a model for estimating the presence of an edge between two nodes.

- Based on the notion of homophily, we can use some *similarity score* between nodes i and j to estimate the probability of e_{ij}.

Your Turn #5

Think up 3 ways to measure the similarity of two nodes, when it is unknown whether an edge exists between them or not.
similarity scores between nodes (when the edge between them is unknown)

Solution

1. Function of node attributes
2. Function of degree
3. Based on overlapping neighborhoods. E.g., Jaccards of neighbors
4. Function of shortest path distance between nodes (1/dist) or (-dist)

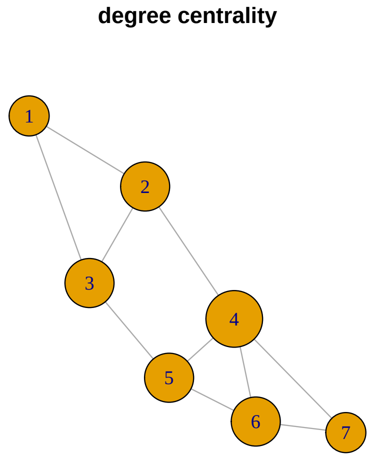
5 Node Importance: Vertex Centrality

Centrality tries to assess how "important" a vertex is.
- Which actors in a social network seem to hold the 'reins of power'?
- How authoritative does a webpage seem to be considered?
- How critical is a router in the internet network?

5.1 Degree centrality

the number of edges (sum of weights) a vertex has is the most basic definition of importance

```
deg = degree(g)
cent.deg = deg/sum(deg)
plot(g, layout=g.layout, vertex.size=80*sqrt(cent.deg))
title("degree centrality")
```



Mathematically, the degree for node i can be written

$$c_i = \sum_j A_{ij}$$

5.2 Closeness centrality

Measures the importance in terms of how 'close' a vertex is to the other vertices in the graph.

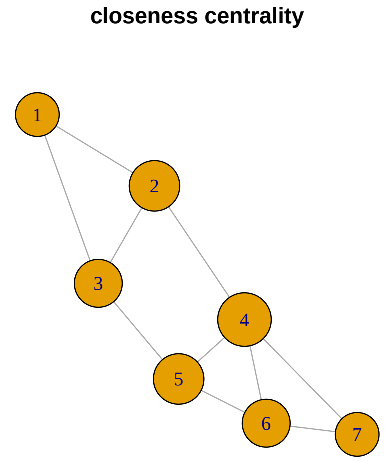
The standard approach is to let the centrality vary inversely with a measure of the total distance of a vertex to all the others:

$$c(v) = \frac{1}{\sum_{u \in V} \text{dist}(v, u)}$$

Closeness is only defined if graph is connected!

```
close = centr_clo(g)$res
cent.close = close/sum(close)
```

```
plot(g, layout=g.layout, vertex.size=80*sqrt(cent.close))
title("closeness centrality")
```



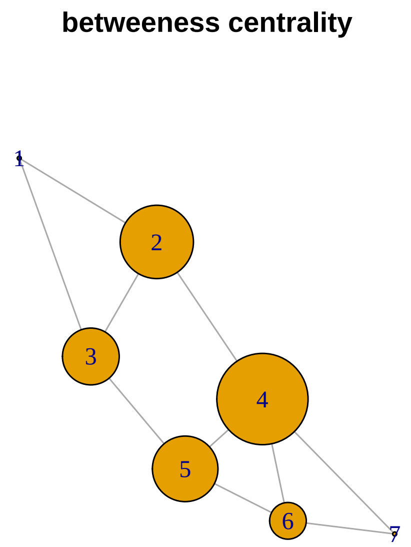
5.3 Betweenness centrality

Measures how many paths cross through a vertex. An important vertex is one in which lots of information flows.

$$c(v) = \sum_{s \neq t \neq v \in V} \frac{\sigma(s,t|v)}{\sigma(s,t)}$$

where $\sigma(s,t|v)$ is the total number of *shortest paths* between s and t that pass through v, and $\sigma(s,t)$ is the total number of shortest paths between s and t (regardless of whether or note they pass through v).

```
between = centr_betw(g)$res
cent.between = between/sum(between)
plot(g,  layout=g.layout, vertex.size=80*sqrt(cent.between))
title("betweeness centrality")
```


betweeness centrality

Centrality scores are commonly standardized so they can be understood relative to the other nodes in the network. Above, I list the centralities as score_i/sum(score), which makes the centralities sum to one over all nodes. In `igraph`, the `centr_<metric>()` functions have an arugment named `normalized=TRUE` which instead divide the score by the theoretical maximum.
You may also see score_i / norm(score), where norm is a vector norm.

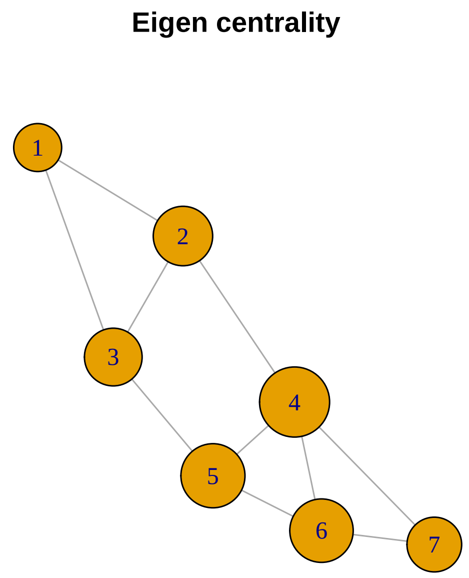
5.4 Eigenvector centrality

Based on the notion that an important vertex will be connected to other importance vertices.

$$c(v) = \alpha \sum_{\{u,v\} \in E} c(u)$$

- Notice that the eigenvector centrality for vertex v is the sum of the centrality of the vertices that it is connected to (scaled by α).
- In a more standard form, $A\mathbf{c} = \lambda\mathbf{c}$, is seen to be the eigen equations for A where $\mathbf{c}$ are the eigenvectors and λ the eigenvalues.
  - If A is not a stochastic matrix (rows sum to one, non-negative), then use the eigenvector corresponding to the largest magnitude eigenvalue
  - Standardize c to either have a maximum value of 1 or norm (sum of squares) of 1.

```r
#eigen = eigen_centrality(g)$vector  # first eigenvalue (max of 1)
eigen = centr_eigen(g)$vector
cent.eigen = eigen/sum(eigen)
plot(g,layout=g.layout,vertex.size=80*sqrt(cent.eigen))
title("Eigen centrality")
```



5.4.1 Power Method

We can use the *power method* to solve $\mathbf{c} = A\mathbf{c}$

$$c^{\text{new}} = Ac^{\text{old}}/||Ac^{\text{old}}||$$

```
A = get.adjacency(g, sparse=FALSE)
n = nrow(A)
y = matrix(1/n, n, 1) # initialize
for (i in 1:50){       # run until converges
  y = A%*%y
  y = y/sum(y)
}
data.frame(cent.eigen, y)
#>   cent.eigen       y
#> 1    0.09121 0.09121
#> 2    0.14012 0.14012
#> 3    0.13214 0.13214
#> 4    0.19490 0.19490
#> 5    0.16308 0.16308
#> 6    0.15973 0.15973
#> 7    0.11881 0.11881
```

6 PageRank

6.1 Random Surfer

The pagerank algorithm is based on the idea of a random (internet) surfer who randomly clicks on links from the current page.

- Consider transforming the adjacency matrix A into the appropriate transition matrix (markov chain)
  - For directed networks
  - Let $P_{ij} = A_{ij}/d_i^{out}$ be the row-standardized transition probability

$$P_{ij} = \begin{cases} \frac{1}{d_i^{out}}, & \text{if } \{i, j\} \in E, \\ 0, & \text{otherwise} \end{cases}$$

  - P_{ij} is the probability of a move from $i \to j$ if all edges are equally likely (random walk)
  - $P = D^{-1}A$ where $D = diag(d^{out})$

```
P = sweep(A, 1, rowSums(A), '/')
round(P, 2)
#>      1    2    3    4    5    6    7
#> 1 0.00 0.50 0.50 0.00 0.00 0.00 0.00
#> 2 0.33 0.00 0.33 0.33 0.00 0.00 0.00
#> 3 0.33 0.33 0.00 0.00 0.33 0.00 0.00
#> 4 0.00 0.25 0.00 0.00 0.25 0.25 0.25
#> 5 0.00 0.00 0.33 0.33 0.00 0.33 0.00
#> 6 0.00 0.00 0.00 0.33 0.33 0.00 0.33
#> 7 0.00 0.00 0.00 0.50 0.00 0.50 0.00
```

6.2 PageRank Details

Consider the directed graph representation of the www: $G = (V, E)$, where $n = |V|$ are the number of webpages

- Webpages link (hyperlink) to other webpages with directed edges
- An important webpage is one that many (important) pages **link to it**
- The PageRank score of page i is

$$\begin{aligned} r_i &= \sum_{\{j,i\} \in E} \frac{r_j}{d_j^{out}} \\ &= \sum_j P_{ji} r_j \end{aligned}$$

- This gives the system of equations

$$\mathbf{r} = P^{\mathsf{T}}\mathbf{r}$$

But we have a problem. What if some pages cannot be reached by other pages?

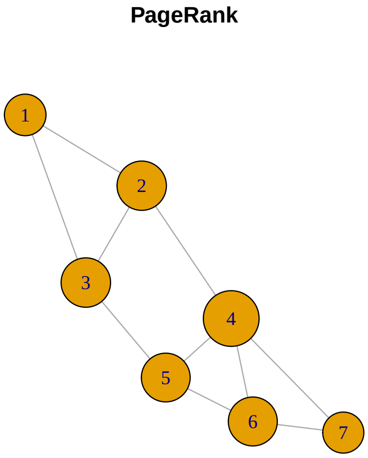
The approach taken in PageRank is to add a dampening factor. Or alternatively the idea that the websurfer will randomly click links, but occasionally will pick another webpage (from the full set of vertices) at random and starts again. This can be modeled by

$$\mathbf{r} = \frac{1-d}{n}\mathbf{e} + dP^{\mathsf{T}}\mathbf{r}$$

- $0 \leq d \leq 1$ is the *dampening factor* or the probability the surfer keeps clicking on the links (and thus $1-d$ the probability of random selection)
  - Original method used $d = 0.85$
- $\mathbf{e}$ is a column vector of ones
- Equivalently,

$$\begin{aligned} r_i &= \frac{1-d}{n} + d \sum_{\{j,i\} \in E} \frac{r_j}{d_j^{out}} \\ &= \frac{1-d}{n} + d \sum_{j=1}^{n} P_{ji} r_j \end{aligned}$$

```
pr = page_rank(g, weights = NA)$vector
cent.pr = pr/sum(pr)
plot(g,layout=g.layout,vertex.size=80*sqrt(cent.pr))
title("PageRank")
```



- The power iteration method can also be used to solve this equation, which finds the eigenvector with eigenvalue of 1. This is a very fast approach which can be parallel processed.

```
P = sweep(A, 1, rowSums(A), '/')
d = 0.85

y = matrix(1/n, n, 1) # initialize
for (i in 1:50){      # run until converges
  y = (1-d)/n + d*crossprod(P,y)
  y = y/sum(y)          # should sum to 1, but roundoff error
}
```

```
data.frame(cent.pr, y)
#>   cent.pr      y
#> 1  0.1069 0.1069
#> 2  0.1505 0.1505
#> 3  0.1512 0.1512
#> 4  0.1920 0.1920
#> 5  0.1470 0.1470
#> 6  0.1482 0.1482
#> 7  0.1042 0.1042
```

7 More Resources

- https://github.com/briatte/awesome-network-analysis
- Two nice R packages to help put graph analysis in the *tidyverse* are:
  - `ggraph`
  - `tidygraph`