



University  
of Manitoba

## Characterising graphs

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The University of Manitoba campuses are located on original lands of Anishinaabeg, Inineew, Anisininew, Dakota and Dene peoples, and on the National Homeland of the Red River Métis.

We respect the Treaties that were made on these territories, we acknowledge the harms and mistakes of the past, and we dedicate ourselves to move forward in partnership with Indigenous communities in a spirit of Reconciliation and collaboration.

# Outline

Why characterise graphs?

A few  $\mathbb{R}$  preliminaries

Measures specific to vertices

Measures at the graph level



Why characterise graphs?

A few R preliminaries

Measures specific to vertices

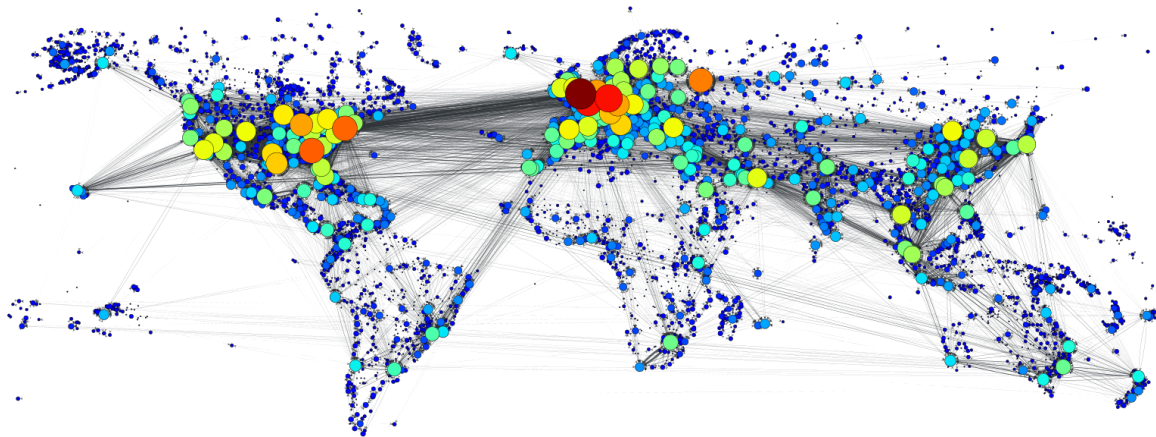
Measures at the graph level

# Why characterise a graph

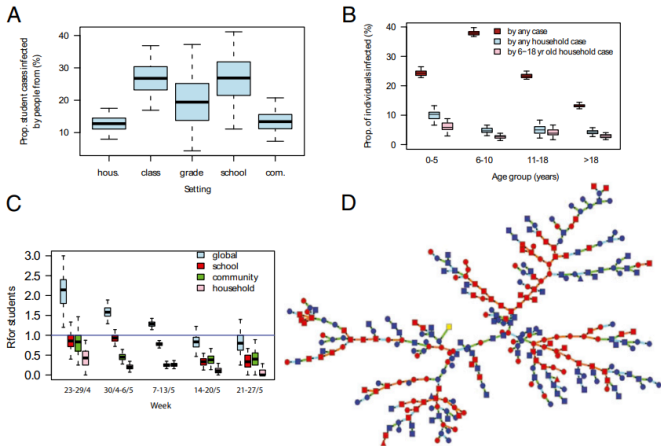
Graphs are everywhere!

To compare graphs, understand their properties, we need ways to describe their shape and characteristics

# The global air transportation network

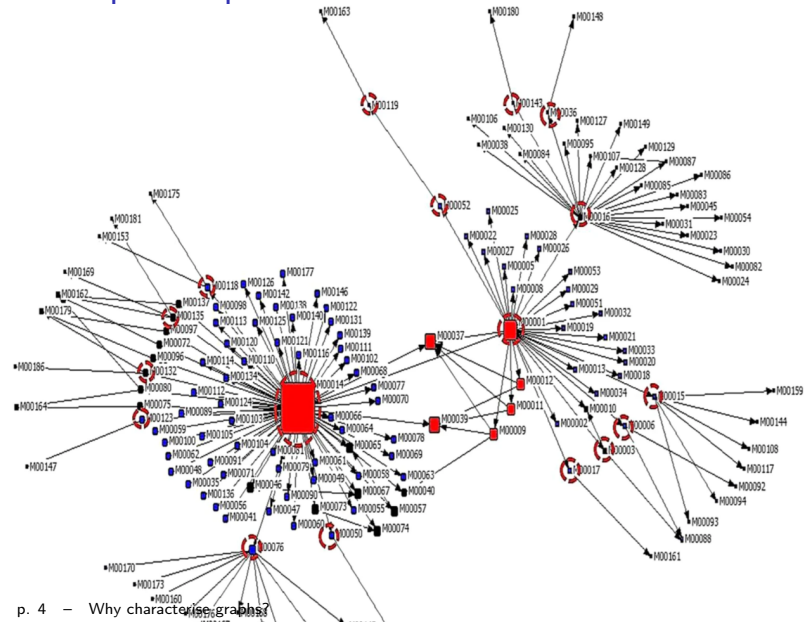


# Example of spread of p-H1N1



**Fig. 4.** Reconstruction of the transmission tree. (A) Proportion of student cases infected by people from their household, class, grade, school, or from the community. (B) Proportion of individuals infected by any other case (red), by any household case (blue), or by a household case aged 6–18 y (pink), as a function of the age of the individual. (C) Weekly estimates of the effective reproduction number in the outbreak (“global” R) and in places (school, household, and community). (D) Reconstructed transmission tree drawn from its predictive distribution (color of the nodes, yellow, first case; red, student of the school; blue, household member of a student; color of the lines for the type of transmission, orange, among students of the school; light blue, among household members; green, in the community; shape of the nodes, circle, female; square, male; triangle, sex is missing). Boxplots give percentiles 2.5%, 25%, 50%, 75%, and 97.5% of the predictive distribution.

# Example of spread of MERS



Topological dynamics of the 2015 South Korea MERS-CoV spread-on-contact networks, Yang & Jung, Scientific Reports 10:4327 (2020)

Some “measures” concern the vertices, others the graph as a whole

In all that follows, unless otherwise indicated,  $G = (V, A)$  is a digraph. If undirected, we write  $G = (V, E)$





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## R packages for analysing graphs

Two main packages: `network` and `igraph`

We will use `igraph`: if you learn how to use it in R, you can easily do the same in Python, C/C++ or Mathematica !

So in the following, I will assume that we have used the command `library(igraph)`

## igraph documentation

These days, there is an issue with the `igraph` documentation site, whereas normally it is quite good

You can find it here

Do read the R vignette, though, as well as the manual

## Setting up a graph

There are multiple ways to set up a graph in `igraph`. Of course, you will need `library(igraph)`

Two main mechanisms:

1. Use a function to create a *known* graph
2. Implement your own graph, describing the vertices and the edges/arcs

## Known graphs (a few)

- ▶ `make_lattice`
- ▶ `make_ring`
- ▶ `make_star`
- ▶ `make_tree`
- ▶ `make_line_graph`
- ▶ `make_full_graph`
- ▶ `make_bipartite_graph`
- ▶ `make_empty_graph`



**Why characterise graphs?**

**A few R preliminaries**

**Measures specific to vertices**

**Measures at the graph level**



## Measures specific to vertices

Centre of a graph

Centrality – Betweenness and closeness

Periphery of a graph

Degree distribution

# Geodesic distance

## Definition 1 (Geodesic distance)

For  $x, y \in V$ , the **geodesic distance**  $d(x, y)$  is the length of the shortest path from  $x$  to  $y$ , with  $d(x, y) = \infty$  if no such path exists

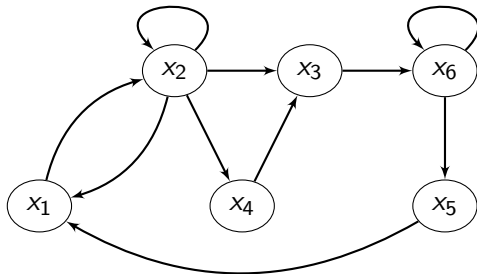


►  $d(x_1, x_2) = 1$

►  $d(x_1, x_3) = 2$

► ...

$$\begin{pmatrix} 0 & 1 & 2 & 2 & 4 & 3 \\ 1 & 0 & 1 & 1 & 3 & 2 \\ 3 & 4 & 0 & 5 & 2 & 1 \\ 4 & 5 & 1 & 0 & 3 & 2 \\ 1 & 2 & 3 & 3 & 0 & 4 \\ 2 & 3 & 4 & 4 & 1 & 0 \end{pmatrix}$$

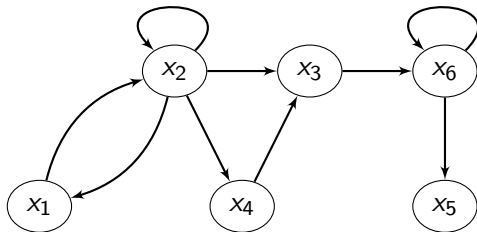


►  $d(x_5, x_1) = \infty$

►  $d(x_3, x_1) = \infty$

► ...

$$\begin{pmatrix} 0 & 1 & 2 & 2 & 4 & 3 \\ 1 & 0 & 1 & 1 & 3 & 2 \\ \infty & \infty & 0 & \infty & 2 & 1 \\ \infty & \infty & 1 & 0 & 3 & 2 \\ \infty & \infty & \infty & \infty & 0 & \infty \\ \infty & \infty & \infty & \infty & 1 & 0 \end{pmatrix}$$



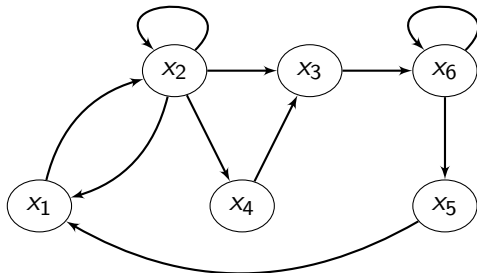
# Eccentricity

## Definition 2 (Vertex eccentricity)

The **eccentricity**  $e(x)$  of vertex  $x \in V$  is

$$e(x) = \max_{\substack{y \in V \\ y \neq x}} d(x, y)$$

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 0 | 1 | 2 | 2 | 4 | 3 |
| 1 | 0 | 1 | 1 | 3 | 2 |
| 3 | 4 | 0 | 5 | 2 | 1 |
| 4 | 5 | 1 | 0 | 3 | 2 |
| 1 | 2 | 3 | 3 | 0 | 4 |
| 2 | 3 | 4 | 4 | 1 | 0 |



## Central points, radius and centre

### Definition 3 (Central point)

A **central point** of  $G$  is a vertex  $x_0$  with smallest eccentricity

### Definition 4 (Radius)

The **radius** of  $G$  is  $\rho(G) = e(x_0)$ , where  $x_0$  is a centre of  $G$ . In other words,

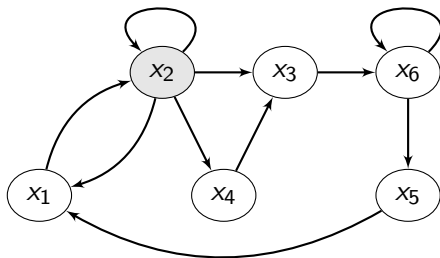
$$\rho(G) = \min_{x \in V} e(x)$$

### Definition 5 (Centre)

The **centre** of  $G$  is the set of vertices that are central points of  $G$ , i.e.,

$$\{x \in V : e(x) = \rho(G)\}$$

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 0 | 1 | 2 | 2 | 4 | 3 |
| 1 | 0 | 1 | 1 | 3 | 2 |
| 3 | 4 | 0 | 5 | 2 | 1 |
| 4 | 5 | 1 | 0 | 3 | 2 |
| 1 | 2 | 3 | 3 | 0 | 4 |
| 2 | 3 | 4 | 4 | 1 | 0 |



Radius is 3,  $x_2$  is a central point (the only one) and the centre is  $\{x_2\}$



## Measures specific to vertices

- Centre of a graph

- Centrality – Betweenness and closeness

- Periphery of a graph

- Degree distribution

## How *central* is a vertex?

*Centrality* tries to answer the question: what are the most influent vertices?

We have seen central vertices and vertices on the periphery, let us consider two other measures of centrality

- ▶ Betweenness centrality
- ▶ Closeness centrality

Many other forms (we will come back to this, e.g., degree centrality)

# Betweenness

## Definition 6 (Betweenness)

$G = (V, A)$  a (di)graph. The **betweenness** of  $v \in V$  is

$$b_D(v) = \sum_{s \neq t \neq v \in V} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

where

- ▶  $\sigma_{st}$  is number of shortest geodesic paths from  $s$  to  $t$
- ▶  $\sigma_{st}(v)$  is number of shortest geodesic paths from  $s$  to  $t$  through  $v$



In other words

- ▶ For each pair of vertices  $(s, t)$ , compute the shortest paths between them
- ▶ For each pair of vertices  $(s, t)$ , determine the fraction of shortest paths that pass through vertex  $v$
- ▶ Sum this fraction over all pairs of vertices  $(s, t)$

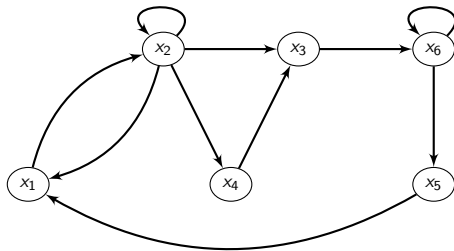
## Normalising betweenness

Betweenness may be normalized by dividing through the number of pairs of vertices not including  $v$ :

- ▶ for directed graphs,  $(n - 1)(n - 2)$
- ▶ for undirected graphs,  $(n - 1)(n - 2)/2$

## Example of betweenness

`distances(G, mode="out")`

$$\begin{pmatrix} 0 & 1 & 2 & 2 & 4 & 3 \\ 1 & 0 & 1 & 1 & 3 & 2 \\ 3 & 4 & 0 & 5 & 2 & 1 \\ 4 & 5 & 1 & 0 & 3 & 2 \\ 1 & 2 & 3 & 3 & 0 & 4 \\ 2 & 3 & 4 & 4 & 1 & 0 \end{pmatrix}$$


## Number of shortest paths

Recall we found `distances(G, mode="out")`

$$\mathcal{D} = \begin{pmatrix} 0 & 1 & 2 & 2 & 4 & 3 \\ 1 & 0 & 1 & 1 & 3 & 2 \\ 3 & 4 & 0 & 5 & 2 & 1 \\ 4 & 5 & 1 & 0 & 3 & 2 \\ 1 & 2 & 3 & 3 & 0 & 4 \\ 2 & 3 & 4 & 4 & 1 & 0 \end{pmatrix}$$

To find the number of shortest paths between pairs of vertices, we can use powers of the adjacency matrix

Write  $\mathcal{D} = [d_{ij}]$ , for a given  $(i, j)$  ( $i \neq j$ ), if  $d_{ij} = k$ , then pick the  $(i, j)$  in  $A^k$

We find

$$\begin{pmatrix} 0 & 1 & 1 & 1 & 1 & 1 \\ 1 & 0 & 1 & 1 & 1 & 1 \\ 1 & 1 & 0 & 1 & 1 & 1 \\ 1 & 1 & 1 & 0 & 1 & 1 \\ 1 & 1 & 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 1 & 1 & 0 \end{pmatrix}$$

Recall that betweenness of  $v$  is

$$b_{\mathcal{D}}(v) = \sum_{s \neq t \neq v \in V} \frac{\sigma_{st}(v)}{\sigma_{st}}$$

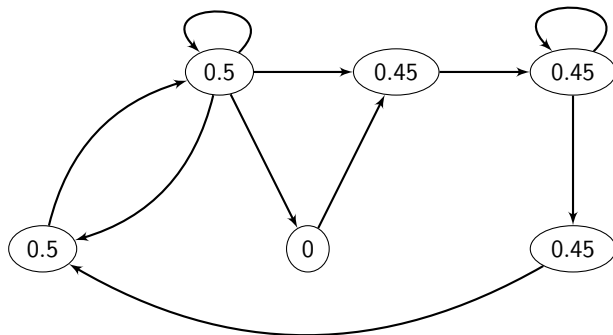
$\sigma_{st}$  (# shortest paths from  $s$  to  $t$ ) is found in the matrix above

What about  $\sigma_{st}(v)$ , # of those shortest paths that go through  $v$ ?

We can use `all_shortest_paths(G, from = s, to = t, mode = "out")`

## Example of betweenness

`betweenness(G, directed = FALSE, normalized = TRUE)`



# Closeness

## Definition 7

$G = (V, A)$ . The **closeness** of  $v \in V$  is

$$c_{\mathcal{D}}(v) = \frac{1}{n-1} \sum_{t \in V \setminus \{v\}} d_{\mathcal{D}}(v, t)$$

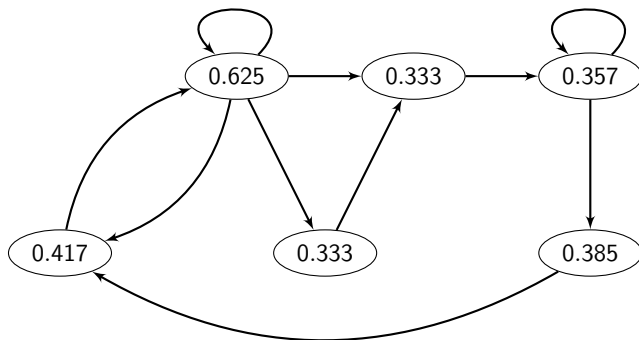
i.e., mean geodesic distance between a vertex  $v$  and all other vertices it has access to

Another definition is

$$c_{\mathcal{D}}(v) = \frac{1}{\sum_{t \in V \setminus \{v\}} d_{\mathcal{D}}(v, t)}$$

## Example of (out) closeness

```
closeness(G, normalized = TRUE, mode='out')
```







## Measures specific to vertices

- Centre of a graph

- Centrality – Betweenness and closeness

- Periphery of a graph

- Degree distribution

# Diameter and periphery of a graph

## Definition 8 (Diameter of a graph)

The **diameter** of  $G$  is

$$\delta(G) = \max_{\substack{x,y \in V \\ x \neq y}} d(x,y) = \max_{x \in V} e(x)$$

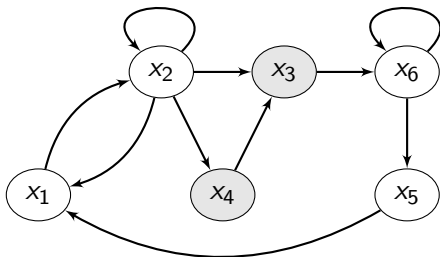
$$\delta(G) < \infty \iff G \text{ strongly connected}$$

## Definition 9 (Periphery)

The **periphery** of a graph is the set of vertices whose eccentricity achieves the diameter, i.e.,

$$\{x \in V : e(x) = \delta(G)\}$$

|   |   |   |   |   |   |
|---|---|---|---|---|---|
| 0 | 1 | 2 | 2 | 4 | 3 |
| 1 | 0 | 1 | 1 | 3 | 2 |
| 3 | 4 | 0 | 5 | 2 | 1 |
| 4 | 5 | 1 | 0 | 3 | 2 |
| 1 | 2 | 3 | 3 | 0 | 4 |
| 2 | 3 | 4 | 4 | 1 | 0 |



Diameter is  $\delta(G) = 5$  and periphery is  $\{x_3, x_4\}$

### Definition 10 (Antipodal vertices)

Vertices  $x, y \in V$  are **antipodal** if  $d(x, y) = \delta(G)$



## Measures specific to vertices

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# Degree distribution

## Definition 11 (Arc incident to a vertex)

If a vertex  $x$  is the initial endpoint of an arc  $u$ , which is not a loop, the arc  $u$  is **incident out of vertex**  $x$

The number of arcs incident out of  $x$  plus the number of loops attached to  $x$  is denoted  $d_G^+(x)$  and is the **outer demi-degree** of  $x$

An arc **incident into vertex**  $x$  and the **inner demi-degree**  $d_G^-(x)$  are defined similarly

## Definition 12 (Degree)

The **degree** of vertex  $x$  is the number of arcs with  $x$  as an endpoint, each loop being counted twice. The degree of  $x$  is denoted  $d_G(x) = d_G^+(x) + d_G^-(x)$

If each vertex has the same degree, the graph is **regular**

### Definition 13 (Isolated vertex)

A vertex of degree 0 is **isolated**.

### Definition 14 (Average degree of $G$ )

$$d(G) = \frac{1}{|V|} \sum_{v \in V} \deg_G(v).$$

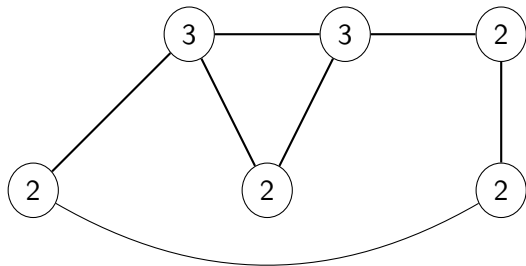
### Definition 15 (Minimum degree of $G$ )

$$\delta(G) = \min\{\deg_G(v) \mid v \in V\}.$$

### Definition 16 (Maximum degree of $G$ )

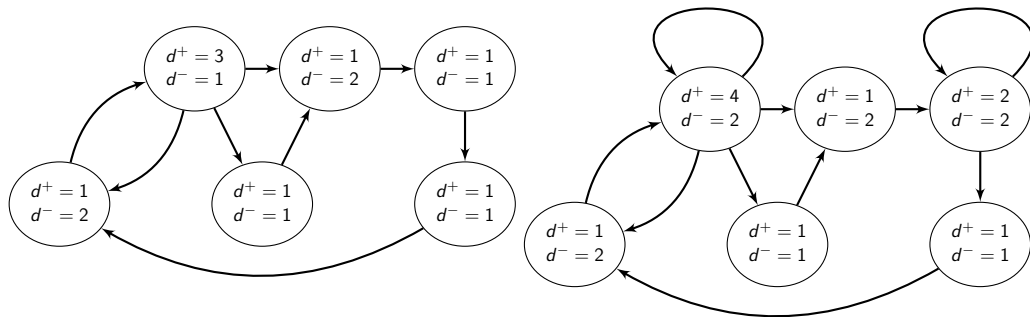
$$\Delta(G) = \max\{\deg_G(v) \mid v \in V\}.$$

## Degrees in an undirected graph



Here, vertices are labelled using the degree

## Degrees in a directed graph





## What to consider about degrees?

Degrees are often considered as a measure of popularity

Often write  $k(i)$  (or  $k_i$ ) for “degree of vertex  $i$ ”,  $k^-(i)$  and  $k^+(i)$  for in- and out-degree

- ▶ Minimum and maximum degree
- ▶ Minimum and maximum in/out-degree. E.g., if you consider the global air transportation network and the in/out-degree of airports, in-degree is a measure of a location’s “popularity” as a travel destination
- ▶ Range of degrees in a graph: are there large discrepancies in connectivity between vertices in the graph?
- ▶ Average degree (often denoted  $\langle k \rangle$  because of physicists)
- ▶ Average in/out-degree
- ▶ Variance of the degrees or in/out-degrees

- ▶ Average (nearest) neighbour degree, to encode for *preferential attachment* (one prefers to hang out with popular people)

$$k_i^{nn} = \frac{1}{k(i)} \sum_{j \in \mathcal{N}(i)} k(j)$$

or, in terms of the adjacency matrix  $A = [a_{ij}]$ ,

$$k_i^{nn} = \frac{1}{k(i)} \sum_j a_{ij} k(j)$$

- ▶ *Excess degree*: take nearest neighbour degree but do not consider the edge/arc followed to get to the neighbour
- ▶ Degree, nearest neighbour and excess degree distributions

## Degrees in igraph

- ▶ `degree` gives the degrees of the vertices
- ▶ `degree_distribution` gives numeric vector of the same length as the maximum degree plus one. The first element is the relative frequency zero degree vertices, the second vertices with degree one, etc.
- ▶ `knn` calculate the average nearest neighbor degree of the given vertices and the same quantity in the function of vertex degree
- ▶ `strength` sums up the edge weights of the adjacent edges for each vertex

## Degree from adjacency matrix

Suppose adjacency matrix take the form  $A = [a_{ij}]$  with  $a_{ij} = 1$  if there is an arc from the vertex indexed  $i$  to the vertex indexed  $j$  and 0 otherwise. (Could be the other way round, using  $A^T$ , just make sure)

Let  $\mathbf{e} = (1, \dots, 1)^T$  be the vector of all ones

$$A\mathbf{e} = (d_G^+(1), \dots, d_G^+(1))^T \text{ (out-degree)}$$

$$\mathbf{e}^T A = (d_G^-(1), \dots, d_G^-(1)) \text{ (in-degree)}$$



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A few R preliminaries

Measures specific to vertices

Measures at the graph level

## Measures at the graph level

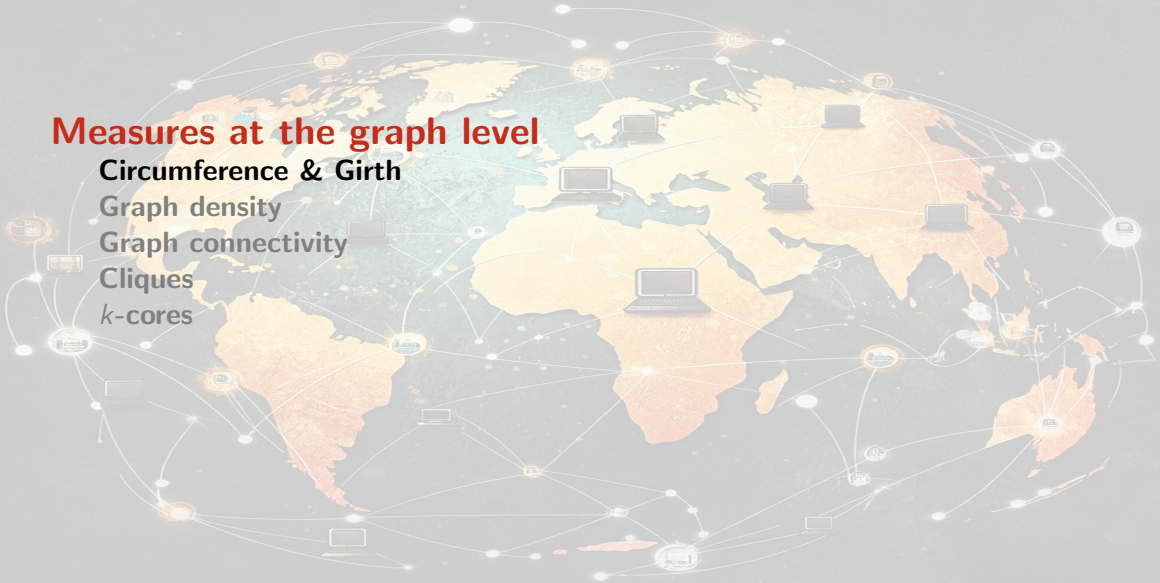
Circumference & Girth

Graph density

Graph connectivity

Cliques

$k$ -cores

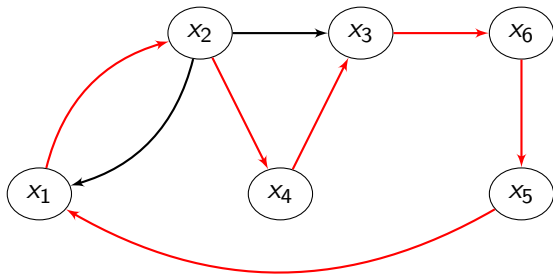


# Circumference

## Definition 17 (Circumference)

In an undirected (resp. directed) graph, the total number of edges (resp. arcs) in the longest cycle of graph  $G$  is the **circumference** of  $G$

Circumference is 6.

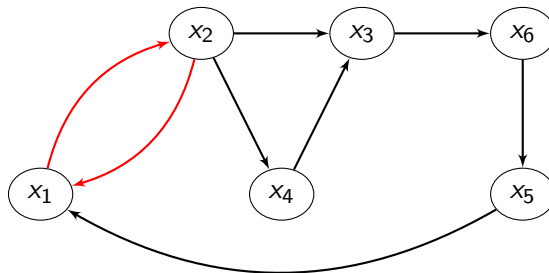


# Girth

## Definition 18 (Girth)

The total number of edges in the shortest cycle of graph  $G$  is the **girth**  $g(G)$

Girth is 2.





## Measures at the graph level

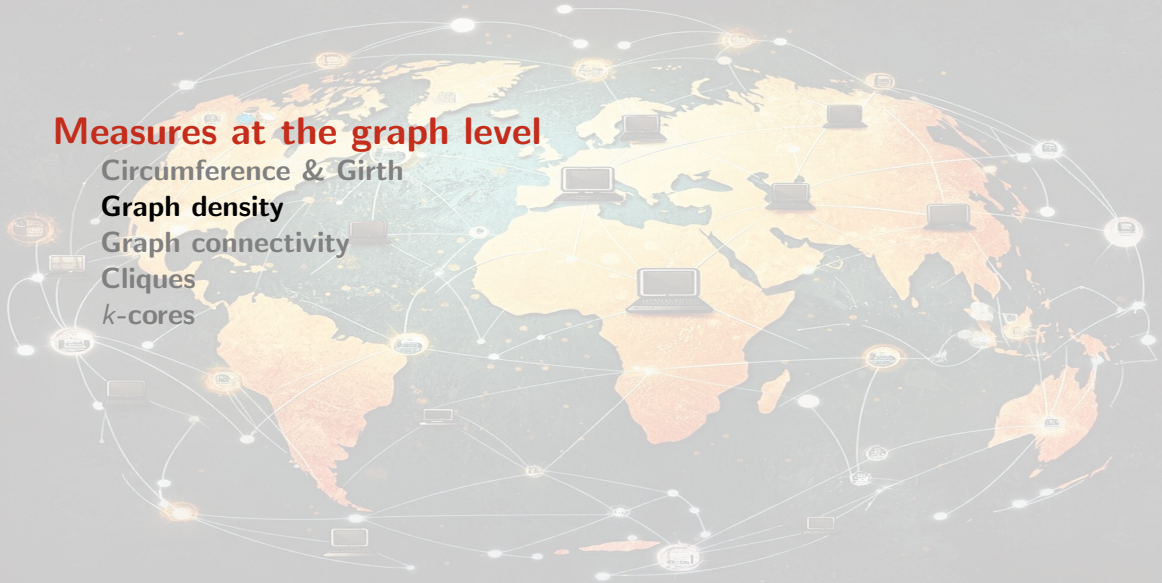
Circumference & Girth

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# Completeness

## Definition 19 (Complete undirected graph)

An undirected graph is complete if every two of its vertices are adjacent.

## Definition 20 (Complete digraph)

A digraph  $D(V, A)$  is complete if  $\forall u, v \in V, uv \in A$ .

In case of simple graphs, completeness effectively means that “information” can be transmitted from every vertex to every other vertex quickly (1 step)

It can be useful to know how far away we are from being complete

## Number of edges/arcs in a complete graph

$G = (V, E)$  undirected and simple of order  $n$  has at most

$$\frac{n(n-1)}{2}$$

edges, while  $G = (V, A)$  directed and simple of order  $n$  has at most

$$n(n-1)$$

arcs

## Density of a graph

### Definition 21 (Density)

The fraction of maximum number of edges or arcs present in the graph is the **density** of the graph.

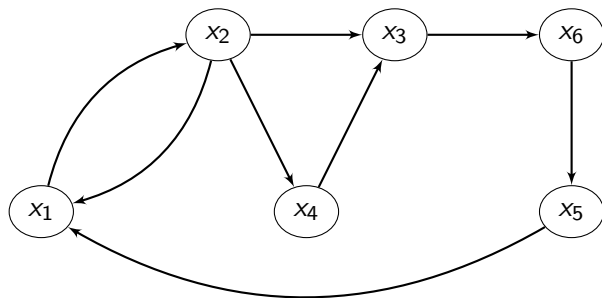
If the graph has  $p$  edges or arcs, then its density is, respectively,

$$\frac{2p}{n(n-1)}$$

or

$$\frac{p}{n(n-1)}$$

## Example of density



Graph has order 6 and thus a max of 30 arcs. Here, 8 arcs  $\Rightarrow$  density 0.267 (26.7% of arcs are present)

## Measures at the graph level

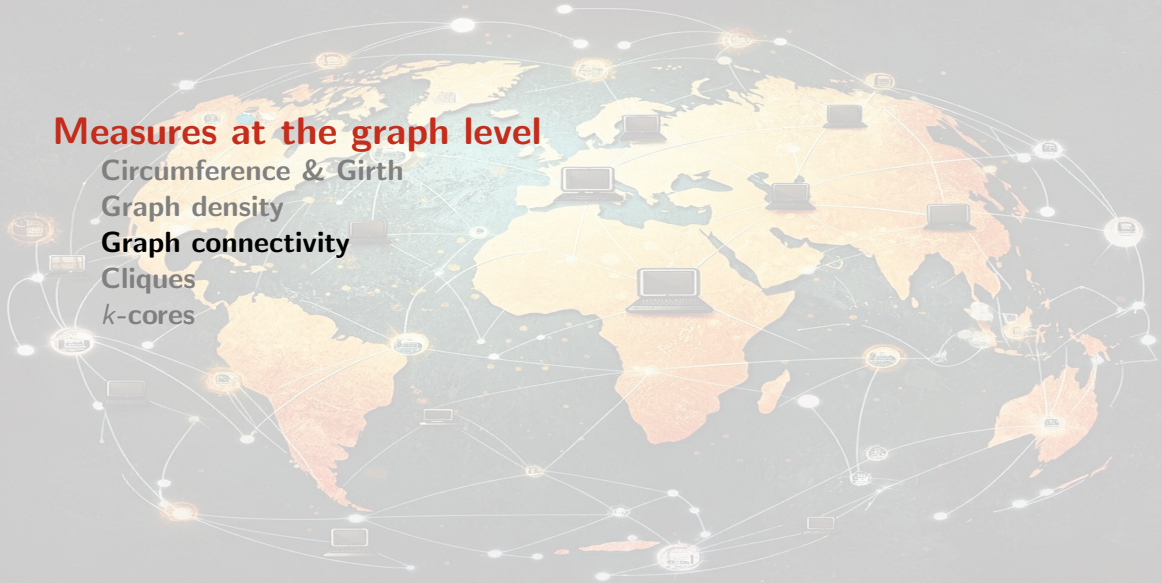
Circumference & Girth

Graph density

Graph connectivity

Cliques

$k$ -cores



# Connectedness

We have already seen connectedness (quasi- or strong in the oriented case)

Connectedness is important in terms of characterising graph properties, as it shows the capacity of the graph to convey information to all the members of the graph (the vertices)

## Definition 22 (Connected graph)

A **connected graph** is a graph that contains a chain  $\mu[x, y]$  for each pair  $x, y$  of distinct vertices

Denote  $x \equiv y$  the relation “ $x = y$ , or  $x \neq y$  and there exists a chain in  $G$  connecting  $x$  and  $y$ ”.  $\equiv$  is an equivalence relation since

1.  $x \equiv y$  [reflexivity]
2.  $x \equiv y \implies y \equiv x$  [symmetry]
3.  $x \equiv y, y \equiv z \implies x \equiv z$  [transitivity]

## Definition 23 (Connected component of a graph)

The classes of the equivalence relation  $\equiv$  partition  $V$  into connected sub-graphs of  $G$  called **connected components**



## Articulation set

### Definition 24 (Articulation set)

For a connected graph, a set  $A$  of vertices is called an **articulation set** (or a **cutset**) if the subgraph of  $G$  generated by  $V - A$  is not connected

`articulation_points(G)` in `igraph` (assumes the graph is undirected, makes it so if not)

## Strongly connected graphs

$G = (V, U)$  connected. A **path of length 0** is any sequence  $\{x\}$  consisting of a single vertex  $x \in V$

For  $x, y \in V$ , let  $x \equiv y$  be the relation “there is a path  $\mu_1[x, y]$  from  $x$  to  $y$  as well as a path  $\mu_2[y, x]$  from  $y$  to  $x$ ”. This is an equivalence relation (it is reflexive, symmetric and transitive)

### Definition 25 (Strong components)

Sets of the form

$$A(x_0) = \{x : x \in V, x \equiv x_0\}$$

are equivalence classes; they partition  $V$  and are the **strongly connected components** of  $G$

### Definition 26 (Strongly connected graph)

$G$  **strongly connected** if it has a single strong component

### Definition 27 (Minimally connected graph)

$G$  is **minimally connected** if it is strongly connected and removal of any arc destroys strong-connectedness

### Definition 28 (Contraction)

$G = (V, U)$ . The **contraction** of the set  $A \subset V$  of vertices consists in replacing  $A$  by a single vertex  $a$  and replacing each arc into (resp. out of)  $A$  by an arc with same index into (resp. out of)  $a$

## Quasi-strong connectedness

### Definition 29 (Quasi-strong connectedness)

$G$  **quasi-strongly connected** if  $\forall x, y \in V$ , exists  $z \in V$  (denoted  $z(x, y)$  to emphasize dependence on  $x, y$ ) from which there is a path to  $x$  and a path to  $y$

Strongly connected  $\implies$  quasi-strongly connected (take  $z(x, y) = x$ ); converse not true

Quasi-strongly connected  $\implies$  connected

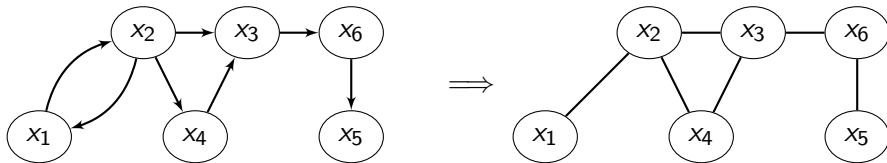
### Lemma 30

$G = (V, U)$  has a root  $\iff G$  quasi-strongly connected

# Weak-connectedness

## Definition 31 (Weakly connected graph)

$G = (V, U)$  **weakly connected** if  $G = (V, E)$  connected, where  $E$  is obtained from  $U$  by ignoring the direction of arcs



## Weak components

Define for  $x, y \in V$  the relation  $x \equiv y$  as “ $x = y$  or  $x \neq y$  and there is a chain in  $G$  connecting  $x$  and  $y$ ” [like for components in an undirected graph, except the graph is directed here]

This defines an equivalence relation

### Definition 32 (Weak components)

Sets of the form

$$A(x_0) = \{x : x \in V, x \equiv x_0\}$$

are equivalence classes partitioning  $V$  into the **weakly connected components** of  $G$

$G = (V, U)$  is weakly connected if there is a single weak component

## Components in igraph

- ▶ `is_connected` decides whether the graph is weakly or strongly connected
- ▶ `components` finds the maximal (weakly or strongly) connected components of a graph
- ▶ `count_components` does almost the same as `components` but returns only the number of clusters found instead of returning the actual clusters
- ▶ `component_distribution` creates a histogram for the maximal connected component sizes
- ▶ `decompose` creates a separate graph for each component of a graph
- ▶ `subcomponent` finds all vertices reachable from a given vertex, or the opposite: all vertices from which a given vertex is reachable via a directed path

## Measures at the graph level

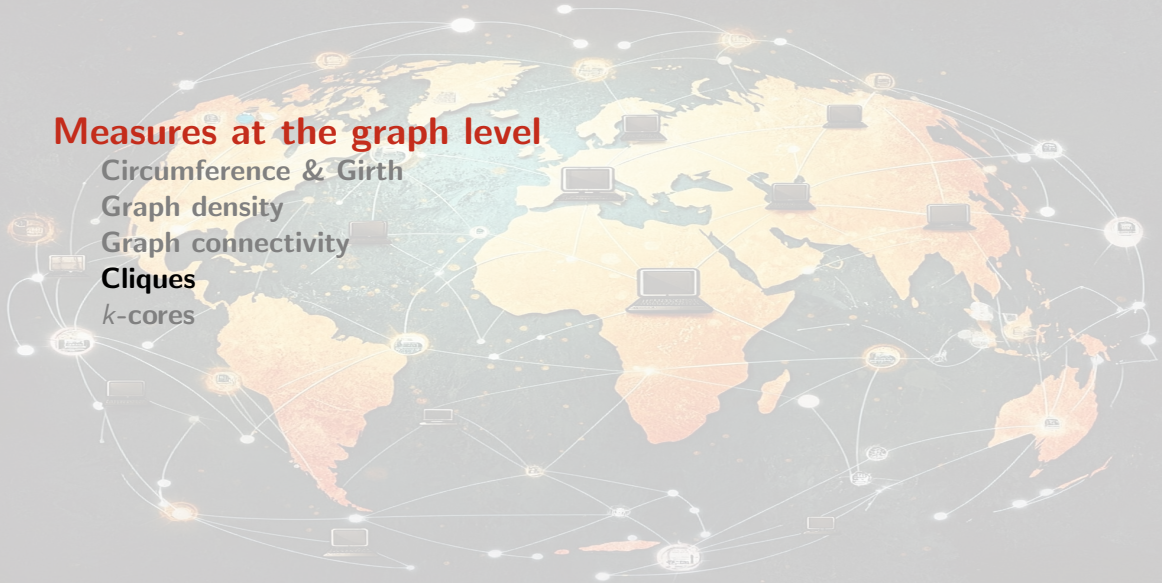
Circumference & Girth

Graph density

Graph connectivity

**Cliques**

*k*-cores





# Cliques

## Definition 33 (Clique in undirected graphs)

$G = (V, E)$  a simple undirected graph. A **clique** is a subgraph  $G'$  of  $G$  such that all vertices in  $G'$  are adjacent

## Definition 34 ( $n$ -clique)

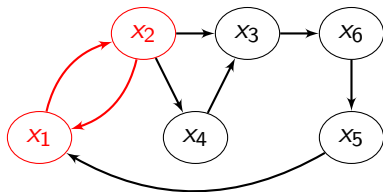
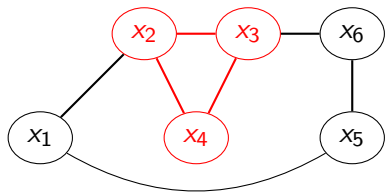
A simple, complete graph on  $n$  vertices is called an  $n$ -**clique** and is often denoted  $K_n$

## Definition 35 (Clique in directed graphs)

$G = (V, U)$  a simple directed graph. A **clique** is a subgraph  $G'$  of  $G$  such that all vertices in  $G'$  are mutually adjacent

## Definition 36 (Maximal clique)

A **maximal clique** is a clique that cannot be extended by adding another adjacent vertex



## Cliques in igraph

- ▶ `cliques` find all complete subgraphs in the input graph, obeying the size limitations given in the `min` and `max` arguments
- ▶ `largest_cliques` finds all largest cliques in the input graph
- ▶ `max_cliques` finds all maximal cliques in the input graph (The largest cliques are always maximal, but a maximal clique is not necessarily the largest)
- ▶ `count_max_cliques` counts the maximal cliques
- ▶ `clique_num` calculates the size of the largest clique(s)

## Measures at the graph level

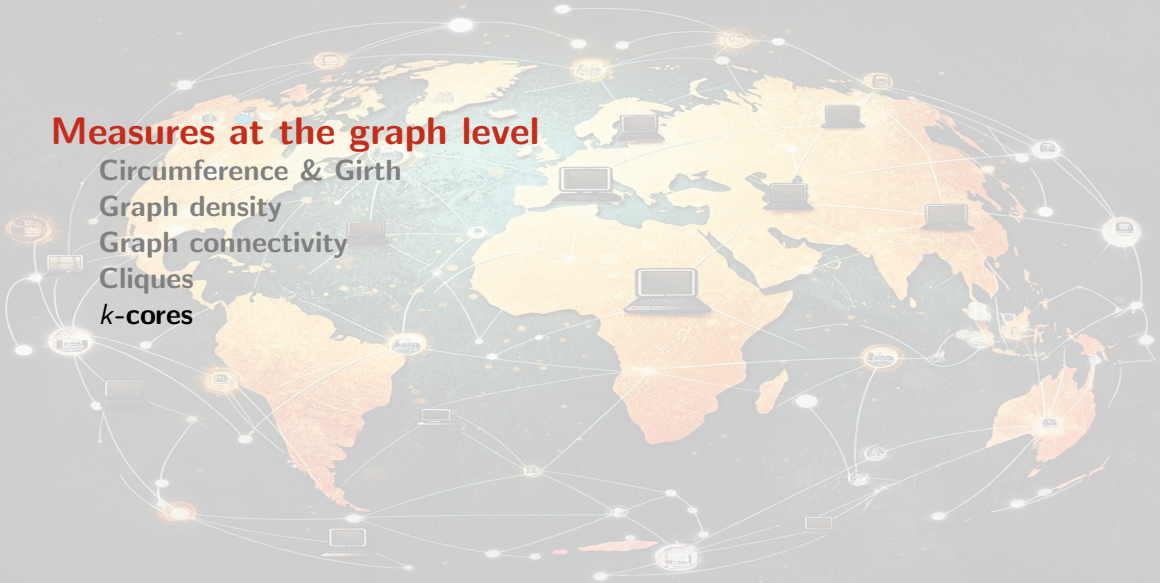
Circumference & Girth

Graph density

Graph connectivity

Cliques

$k$ -cores



## $k$ -core

### Definition 37 ( $k$ -core of a graph)

$G = (V, U)$  a graph. The **k-core** of  $G$  is a maximal subgraph in which each vertex has degree at least  $k$

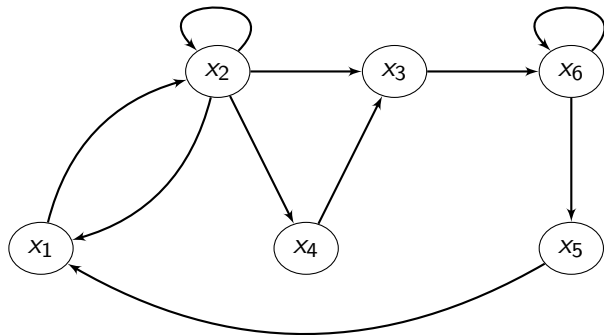
### Definition 38 (Coreness of a vertex)

$G = (V, U)$  a graph,  $x \in V$ . The **coreness** of  $x$  is  $k$  if  $x$  belongs to the  $k$ -core of  $G$  but not to the  $k + 1$  core of  $G$

For directed graphs, in-cores or out-cores depending on whether in-degree or out-degree is used

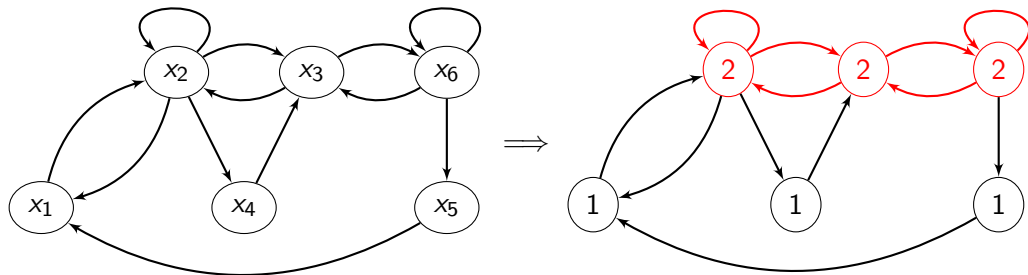
In igraph: `coreness`

## Coreness in the directed case



$G$  has only a 1-in-core and 1-out-core: there is no (maximal) subgraph in which the in- or out-degree is larger than 1

## In-coreness in the directed case



## Coreness in the undirected case

