

Barbara Ikica

Computational Social Science seminar

29 October 2019

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Motivation

Outline

Network algorithms

Data representation Computational complexit

Examples

Centrality indices [PR] Community detection [mPW]

References

Software Reading

Main ingredients

Algorithm

"A set of mathematical instructions or rules that, especially if given to a computer, will help to calculate an answer to a problem."

(Cambridge Dictionary)



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"A set of mathematical instructions or rules that, especially if given to a computer, will help to calculate an answer to a problem."

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Network

"A network is, in its simplest form, a collection of points joined together in pairs by lines." (Newman, Networks: An Introduction, 2010)

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Königsberg bridge problem



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Königsberg bridge problem

Does there exist a route that crosses each of the seven bridges exactly once?



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Meanwhile, in Zürich ...



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- Centrality indices PageRank
- Community detection the modified Petford–Welsh algorithm



Adjacency matrix

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$$A_{ij} = \left\{ \begin{array}{ll} 1; & ij \in E, \\ 0; & \text{otherwise.} \end{array} \right.$$

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Adjacency matrix

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$A_{ij} = \begin{cases} 1; \\ 0; \end{cases}$	$ij \in E$, otherwise.
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Adjacency list



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Adjacency list



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Alternatives

- **Adjacency trees** (quick performance on average)
- Edge lists (compact representation)
- Binary heaps (efficient storage of values/weights)

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Complexity

Computational complexity

Computational resources (time, space, memory) needed to run an algorithm.

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Time complexity

An estimate how the running time scales with the input.

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Computational resources (time, space, memory) needed to run an algorithm.

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An estimate how the running time scales with the input.

Example: finding the highest degree

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Vertex degrees: 5 3

3 3

Current highest degree: 0

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Vertex degrees:



Current highest degree:

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Vertex degrees:



Current highest degree: 5

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Example: finding the highest degree

Vertex degrees:533Current highest degree:5

3

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Complexity

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Computational resources (time, space, memory) needed to run an algorithm.

Time complexity

An estimate how the running time scales with the input.

Example: finding the highest degree

Vertex degrees: Highest degree:

5 3 3 3 5

Time complexity:



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Complexity

Computational complexity

Computational resources (time, space, memory) needed to run an algorithm.

Time complexity

An estimate how the running time scales with the input.

Example: $\mathcal{O}(|V|^4)$

 |V|
 Running time

 1000 (test network)
 1 second

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An estimate how the running time scales with the input.

Example: $\mathcal{O}(|V|^4)$

V	Running time
1000 (test network)	1 second
10^{6}	pprox 30,000 years

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Computational resources (time, space, memory) needed to run an algorithm.

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An estimate how the running time scales with the input.

Example: $\mathcal{O}(|V|^4)$





Key takeaway

Always pre-estimate the running time (test run first, scale up appropriately).

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Closeness centrality

Centrality index

A measure of *importance*, *influence*, or *power* of a vertex/edge in a network.

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Centrality index

A measure of *importance*, *influence*, or *power* of a vertex/edge in a network.

Service facility location problem

Closeness centrality

Where should we place a shopping mall to minimise the total distance to all customers in the region?
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Service facility location problem

Closeness centrality

Where should we place a shopping mall to minimise the total distance to all customers in the region?

Closeness centrality

$$c_C(u) = \left(\sum_{v \in V} d(u, v)\right)^{-1}$$



Breadth-first search

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$$-1$$
 0 -1 1 -1 1 -1 1 -1 2 2 -1 -1

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 $\begin{bmatrix} -1 & 0 & -1 & 1 & -1 & 1 & -1 & -1 & 2 & 2 & 3 & 3 \end{bmatrix}$

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 $\begin{bmatrix} -1 & 0 & -1 & 1 & -1 & 1 & -1 & -1 & 2 & 2 & 3 & 3 \end{bmatrix}$

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Breadth-first search

• Recovers connected components

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- Recovers connected components
- Can be easily extended to find the corresponding shortest paths as well

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- Recovers connected components
- Can be easily extended to find the corresponding shortest paths as well
- Naïve implementation: O(|V| + r|V| + |V| · |E|/|V|) (worst case: r = n; most networks in practice: r = log n)

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- Recovers connected components
- Can be easily extended to find the corresponding shortest paths as well
- Naïve implementation: $\mathcal{O}(|V| + r|V| + |V| \cdot |E|/|V|)$ (worst case: r = n; most networks in practice: $r = \log n$)
- Optimised code: $\mathcal{O}(|V| + |V| \cdot |E|/|V|)$ (sparse networks: $\mathcal{O}(|V|)$, dense networks: $\mathcal{O}(|V|^2)$)

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- Optimised code: $\mathcal{O}(|V| + |V| \cdot |E|/|V|)$ (sparse networks: $\mathcal{O}(|V|)$, dense networks: $\mathcal{O}(|V|^2)$)
- Closeness centrality $c_C(u)$ for $u \in V$: $\mathcal{O}(|V| + |E|)$

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- Optimised code: $\mathcal{O}(|V| + |V| \cdot |E|/|V|)$ (sparse networks: $\mathcal{O}(|V|)$, dense networks: $\mathcal{O}(|V|^2)$)
- Closeness centrality $c_C(u)$ for $u \in V$: $\mathcal{O}(|V| + |E|)$
- Shortest paths on weighted networks: Dijkstra's algorithm

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PageRank

PageRank

$$c_{\mathrm{PR}}(u) = d \sum_{v \in \mathcal{N}^{-}(u)} \frac{c_{\mathrm{PR}}(v)}{\deg^{+}(v)} + (1-d)$$

Brin, S. & Page, L. The Anatomy of a Large-Scale Hypertextual Web Search Engine. *Computer Networks and ISDN Systems* **30**(1–7) (1998), 107–117.



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Motivation for the mPW algorithm

A proper colouring is an assignment of colours to the vertices of a graph so that no two adjacent vertices have the same colour, i.e., $c: V \to \{1, 2, ..., k\}$ s.t. $c(i) \neq c(j)$ for all $ij \in E$.

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Petford–Welsh algorithm

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Petford–Welsh algorithm

Petford, A. D. & Welsh, D. J. A. A Randomised 3-Colouring Algorithm, *Discrete Math.* **74** (1989), 253–261.

Žerovnik, J. A Randomized Algorithm for *k*-Colorability, *Discrete Math.* **131** (1994), 379–393.

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A randomised k-colouring algorithm

1. get initial k-colouring



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Petford–Welsh algorithm

- 1. get initial k-colouring
- 2. while (there is a bad vertex) and (not too many steps) repeat



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- 1. get initial k-colouring
- 2. while (there is a bad vertex) and (not too many steps) repeat
 - 2.1 choose a bad vertex v uniformly at random



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Petford–Welsh algorithm

- 1. get initial k-colouring
- 2. while (there is a bad vertex) and (not too many steps) repeat
 - $2.1\;$ choose a bad vertex v uniformly at random
 - 2.2 choose a new colour *i* for *v* proportionally to $\omega^{-\mathcal{N}(v,i)}$ where $\omega > 1$ and $\mathcal{N}(v,i) = \#$ neighbours of *v* of colour *i*



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$\mathcal{N}(9,r) = 1$
$\mathcal{N}(9,b) = 2$
$\mathcal{N}(9,y) = 0$
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 - $2.1\;$ choose a bad vertex v uniformly at random
 - 2.2 choose a new colour i for v proportionally to $\omega^{-\mathcal{N}(v,i)}$ where $\omega > 1$ and $\mathcal{N}(v,i) = \#$ neighbours of v of colour i



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- 1. get initial k-colouring
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Petford–Welsh algorithm

The Petford-Welsh algorithm ...

- ... mimics the behaviour of a physical process based on a multi-particle system in statistical mechanics (*the antivoter model* by Donnely and Welsh),
- ... acts locally; thus, it is highly parallelisable,
- ... has the weak convergence property: If $k > \chi(G)$, there is a positive probability that the algorithm finds a proper k-colouring in a finite number of steps (regardless of the initial colouring).

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Proposition

A suitably defined parallel variant of the algorithm with a positive probability finds a proper colouring in one (parallel) step starting from any initial colouring, provided that a proper colouring exists.

Consequence

If we increase the number of steps of the algorithm, the probability of reaching a proper colouring becomes as close to 1 as desired.

Žerovnik, J. & Kaufman, M. A parallel variant of a heuristical algorithm for graph coloring – Corrigendum, *Parallel Comput.* **18** (1993), 897–900.

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Clustering

Partitioning or grouping data into "similar" subsets.

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Clustering

A partitioning clustering method separates a given set of objects $X = \{x_1, x_2, \dots, x_n\}$ into non-overlapping groups/clusters $C = \{C_1, C_2, \dots, C_m\}$ that satisfy

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A partitioning clustering method separates a given set of objects $X = \{x_1, x_2, \dots, x_n\}$ into non-overlapping groups/clusters $C = \{C_1, C_2, \dots, C_m\}$ that satisfy

•
$$C_i \neq \emptyset$$
 for all $1 \le i \le m$,

•
$$\cup_{i=1}^m C_i = X$$
,

•
$$C_i \cap C_j = \emptyset$$
 for all $1 \le i < j \le m$.

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A randomised *clustering* algorithm [https://github.com/ikicab/mPW]

1. get initial k-clustering



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A randomised *clustering* algorithm [https://github.com/ikicab/mPW]

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An adaptation of the Petford–Welsh algorithm

- 1. get initial k-clustering
- 2. while (there is a *bad vertex*) and ($Var[bad edges] \ge tol$) repeat



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 - $2.1 \;$ choose a bad vertex v uniformly at random



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Stopping condition

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Run 1 Run 2 500 Run 3 Run 4 Run 5 400 Run 6 Bad edges Run 7 300 Run 8 Run 9 Run 10 200 100 ò 100 200 300 400 500 Iteration step

 $\mathrm{Var}\left(\texttt{bad_edges}\left[\texttt{step}-l+1:\texttt{step}\right]\right) < \texttt{tol}$
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• different clusters get assigned the same colour due to random seeds



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• different clusters get assigned the same colour due to random seeds [Average co-membership matrix: for each clustering solution c, $C_c(i, j) = 1$ iff i and j belong to the same cluster (else 0)]



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Internal indices

The clustering is judged on the basis of certain intrinsic statistical properties of the clustering itself.

Modularity, conductance, coverage

Quality measures

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Internal indices

The clustering is judged on the basis of certain intrinsic statistical properties of the clustering itself.

Modularity, conductance, coverage

External indices

The clustering is compared to a user-given gold-standard clustering (using a pairwise/mapping approach).

Normalised mutual information, adjusted mutual information, adjusted Rand index, F_{β} score, Fowlkes–Mallows index, Jaccard index, V-measure

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Quality measures / Internal indices

Modularity

$$\boxed{Q = \frac{1}{2|E|} \sum_{u,v \in V} \left(a_{uv} - \frac{k_u k_v}{2|E|} \right) \delta(c_u, c_v)}$$

Compares the presence of each intra-cluster edge with the probability of this edge in a random graph

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Quality measures / Internal indices

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Compares the presence of each intra-cluster edge with the probability of this edge in a random graph

Coverage

$$\gamma = \frac{\sum_{u,v \in V} a_{uv} \delta(c_u, c_v)}{\sum_{u,v \in V} a_{uv}}$$

A measure of intra-cluster density

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Quality measures / Internal indices

Conductance

$$\phi = 1 - \frac{1}{|\mathcal{C}|} \sum_{C_i \in \mathcal{C}} \phi(C_i)$$

$$\phi(C_i) = \frac{\sum_{u \in C_i, v \notin C_i} a_{uv}}{\min\left\{\sum_{u \in C_i, v \in V} a_{uv}, \sum_{u \notin C_i, v \in V} a_{uv}\right\}}$$

A measure of inter-cluster sparsity

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Quality measures / External indices

Normalized mutual information

$$\mathrm{NMI}(\mathcal{C},\mathcal{G}) = \frac{\mathrm{MI}(\mathcal{C},\mathcal{G})}{\sqrt{\mathrm{H}(\mathcal{C})\mathrm{H}(\mathcal{G})}}$$

$$\begin{split} \mathrm{MI}(\mathcal{C},\mathcal{G}) &= \mathrm{H}(\mathcal{C}) + \mathrm{H}(\mathcal{G}) - \mathrm{H}(\mathcal{C},\mathcal{G}) \\ \mathrm{H}(\mathcal{C}_i) &= -\sum_{C \in \mathcal{C}_i} \frac{|C|}{|V|} \log \frac{|C|}{|V|} \\ \mathrm{H}(\mathcal{C},\mathcal{G}) &= -\sum_{C_i \in \mathcal{C}, G_i \in \mathcal{G}} \frac{|C_i \cap G_j|}{|V|} \log \frac{|C_i \cap G_j|}{|V|} \end{split}$$

A measure of "information overlap" between ${\mathcal C}$ and ${\mathcal G}$

Quality measures / External indices

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Adjusted mutual information
$$AMI = \frac{MI(\mathcal{C}, \mathcal{G}) - \mathbb{E}[MI(\mathcal{C}, \mathcal{G})]}{\sqrt{H(\mathcal{C})H(\mathcal{G})} - \mathbb{E}[MI(\mathcal{C}, \mathcal{G})]}$$

A measure of "information overlap" between ${\mathcal C}$ and ${\mathcal G}$ adjusted for chance

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Adjusted Rand index

$$ARI(\mathcal{C},\mathcal{G}) = \frac{RI(\mathcal{C},\mathcal{G}) - E[RI(\mathcal{C},\mathcal{G})]}{\max(RI(\mathcal{C},\mathcal{G})) - E[RI(\mathcal{C},\mathcal{G})]} = \frac{2(TP \cdot TN - FP \cdot FN)}{(TN + FP)(FP + TP) + (TN + FN)(FN + TP)}$$

A measure of the level of agreement between ${\cal C}$ and ${\cal G}$ as the fraction of agreeing pairs of vertices to all possible pairs of vertices

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F_{β} score

$$F_{\beta} = \frac{(1+\beta^2) \cdot TP}{(1+\beta^2) \cdot TP + \beta^2 \cdot FN + FP}$$

Weighted harmonic mean of precision and recall

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Quality measures / External indices

F_{β} score

$$F_{\beta} = \frac{(1+\beta^2) \cdot TP}{(1+\beta^2) \cdot TP + \beta^2 \cdot FN + FP}$$

Weighted harmonic mean of precision and recall

Fowlkes-Mallows index

$$\mathrm{FM} = \sqrt{\frac{TP}{TP + FP} \cdot \frac{TP}{TP + FN}}$$

Geometric mean of precision and recall

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Jaccard index

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Jaccard index

$$F_{\beta} = \frac{(1+\beta^2) \cdot TP}{(1+\beta^2) \cdot TP + \beta^2 \cdot FN + FP}$$

V-measure

$$\mathbf{V}_{\beta} = (1+\beta) \frac{ho \cdot cp}{\beta \cdot ho + cp}$$

Harmonic mean of homogeneity $h\boldsymbol{o}$ and completeness cp of the clustering solution

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Experiments

Zachary (|V| = 34, |E| = 78)

Ties amongst the members of a university karate club by Wayne Zachary.



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Experiments / Zachary's karate club

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Method	NMI	ARI	ϕ	γ	Q	$ \mathcal{C} $
Edge bet.	0.517	0.392	0.424	0.692	0.401	5
Fastgreedy	0.576	0.568	0.574	0.756	0.381	3
Infomap	0.578	0.591	0.668	0.821	0.402	3
Label prop.	0.865	0.882	0.773	0.949	0.415	3
Leading eig.	0.612	0.435	0.487	0.667	0.393	4
Multilevel	0.516	0.392	0.558	0.731	0.419	4
Spinglass	0.627	0.509	0.563	0.756	0.420	4
Walktrap	0.531	0.321	0.434	0.590	0.353	5
mPW	1.000	1.000	0.773	0.949	0.403	2

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UK faculty (|V| = 34, |E| = 78)

The personal friendship network of a faculty of a UK university; the school affiliation of each individual is stored as a vertex attribute.



Experiments / UK faculty

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Method	NMI	ARI	ϕ	γ	Q	$ \mathcal{C} $
Edge bet.	0.796	0.825	0.513	0.827	0.413	4
Fastgreedy	0.849	0.820	0.553	0.775	0.444	4
Infomap	0.862	0.875	0.709	0.841	0.432	3
Label prop.	0.862	0.875	0.709	0.953	0.432	3
Leading eig.	0.863	0.871	0.488	0.768	0.397	4
Multilevel	0.802	0.796	0.573	0.749	0.449	4
Spinglass	0.872	0.842	0.573	0.749	0.449	4
Walktrap	0.862	0.875	0.709	0.841	0.432	3
mPW	0.911	0.918	0.741	0.953	0.432	3

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American college football (|V| = 115, |E| = 613)

A network of regular season games between teams divided into 12 conferences.



Experiments / American college football

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Method	NMI	ARI	ϕ	γ	Q	$ \mathcal{C} $
Edge bet.	0.880	0.778	0.533	0.710	0.600	10
Fastgreedy	0.708	0.474	0.567	0.731	0.550	6
Multilevel	0.891	0.807	0.547	0.708	0.605	10
Leading eig.	0.703	0.464	0.456	0.641	0.493	8
Infomap	0.924	0.897	0.505	0.690	0.601	12
Label prop.	0.927	0.889	0.568	0.741	0.605	11
Spinglass	0.929	0.900	0.563	0.728	0.605	11
Walktrap	0.888	0.815	0.547	0.705	0.603	10
mPW	0.936	0.900	0.600	0.780	0.603	9

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Political blogs (|V| = 1222, |E| = 16714)

Interactions between liberal and conservative blogs over the period of two months preceding the U.S. Presidential Election of 2004.

Method	NMI	ARI	ϕ	γ	Q	$ \mathcal{C} $
Edge bet.	_	_	_	_	_	_
Fastgreedy	0.659	0.785	0.451	0.923	0.427	10
Infomap	0.523	0.651	0.250	0.899	0.423	41
Label prop.	0.723	0.813	0.857	1.000	0.426	3
Leading eig.	0.693	0.781	0.854	0.926	0.424	2
Multilevel	0.651	0.774	0.476	0.920	0.427	9
Spinglass	0.649	0.783	0.315	0.922	0.427	15
Walktrap	0.646	0.760	0.484	0.925	0.425	11
mPW	0.732	0.820	0.857	0.927	0.426	4

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International E-road network (|V| = 1040, |E| = 1305)

An international system for numbering and designating roads stretching throughout Europe and some parts of Central Asia.



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An international system for numbering and designating roads stretching throughout Europe and some parts of Central Asia.



Experiments / International E-road network

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Method	ϕ	γ	Q	$ \mathcal{C} $
Edge bet.	_	_	_	_
Fastgreedy	0.860	0.917	0.861	24
Infomap	0.663	0.787	0.777	126
Label prop.	0.731	0.856	0.828	82
Leading eig.	0.794	0.887	0.835	26
Multilevel	0.873	0.921	0.867	24
Spinglass	0.866	0.924	0.872	25
Walktrap	0.757	0.886	0.828	67
mPW	0.945	0.979	0.845	17

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U.S. airports (|V| = 745, |E| = 4618)

A network of flights between U.S. airports.


Experiments / U.S. airports

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Method	ϕ	γ	Q	$ \mathcal{C} $
Edge bet.	0.155	0.932	0.314	118
Fastgreedy	0.594	0.771	0.431	18
Infomap	0.477	0.913	0.310	49
Label prop.	0.653	0.959	0.258	20
Leading eig.	0.682	0.806	0.410	3
Multilevel	0.617	0.790	0.441	16
Spinglass	0.586	0.773	0.441	17
Walktrap	0.342	0.788	0.337	84
mPW	0.774	0.976	0.285	13

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Experiments / Normalised mutual information



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Experiments / Adjusted mutual information



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Experiments / Conductance

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Experiments / Coverage

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Experiments / Modularity

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LFR benchmark

$$\mathrm{LFR}(|V| = 1000, \gamma = 2, \beta = 1, \texttt{k_avg} = 15, \texttt{k_max} = 100, \texttt{c_min} = 50, \texttt{c_max} = 100)$$



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LFR benchmark

$$\mathrm{LFR}(|V|=1000, \gamma=3, \beta=2, \texttt{k_avg}=15, \texttt{k_max}=50)$$





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LFR benchmark

$$\mathrm{LFR}(|V|=1000, \gamma=2, \beta=1, \texttt{k_avg}=25, \texttt{k_max}=150)$$



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Computer resources

Network analysis and visualisation software

- Pajek (free; large network analysis): http://vlado.fmf.uni-lj.si/pub/networks/pajek/
- Gephi (free; (dynamic) network visualisation): https://gephi.org/
- igraph (free; R/Python/Mathematica/C/C++ network analysis package): https://igraph.org/
- NetworkX (free; Python package for complex networks): https://networkx.github.io/
- SNAP (free; Python/C++ high performance library for large networks): http://snap.stanford.edu/
- Mathematica (commercial): https://reference.wolfram.com/language/guide/GraphsAndNetworks.html
- MATLAB (commercial): https://mathworks.com/help/matlab/graph-and-network-algorithms.html

Network datasets

- Newman: http://www-personal.umich.edu/~mejn/netdata/
- Koblenz Network Collection: http://konect.uni-koblenz.de/networks/
- SuiteSparse Matrix Collection: https://sparse.tamu.edu/
- Network Repository: http://networkrepository.com/
- (BIO)SNAP: http://snap.stanford.edu/data/index.html

Reading

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- Brandes, U. & Erlebach, T. *Network Analysis: Methodological Foundations* (Springer, Berlin, Heidelberg, 2005).
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