Learning from Networks

Graph Analytics: Node-Level

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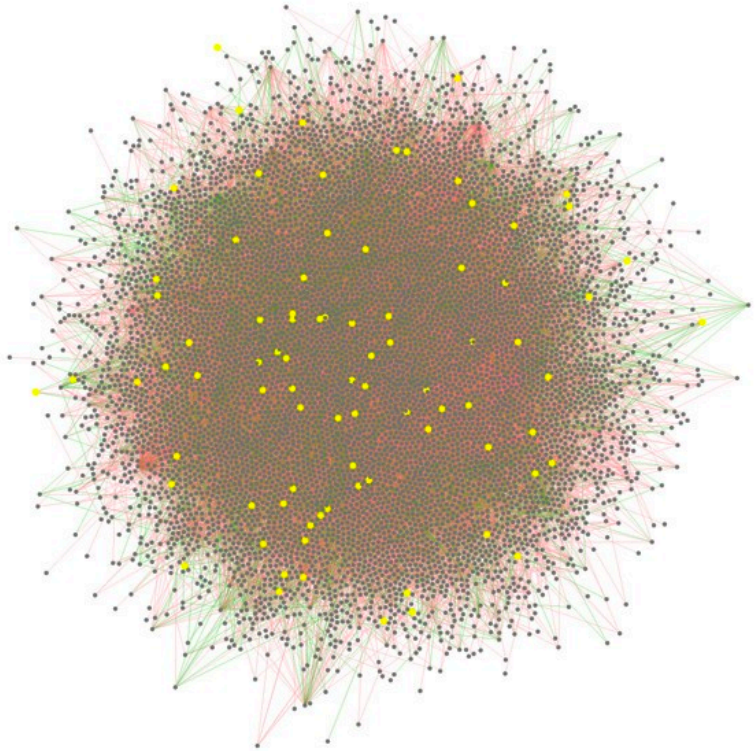
Motivation

In several applications: interested in computing some *scores of importance for nodes* based on the network structure

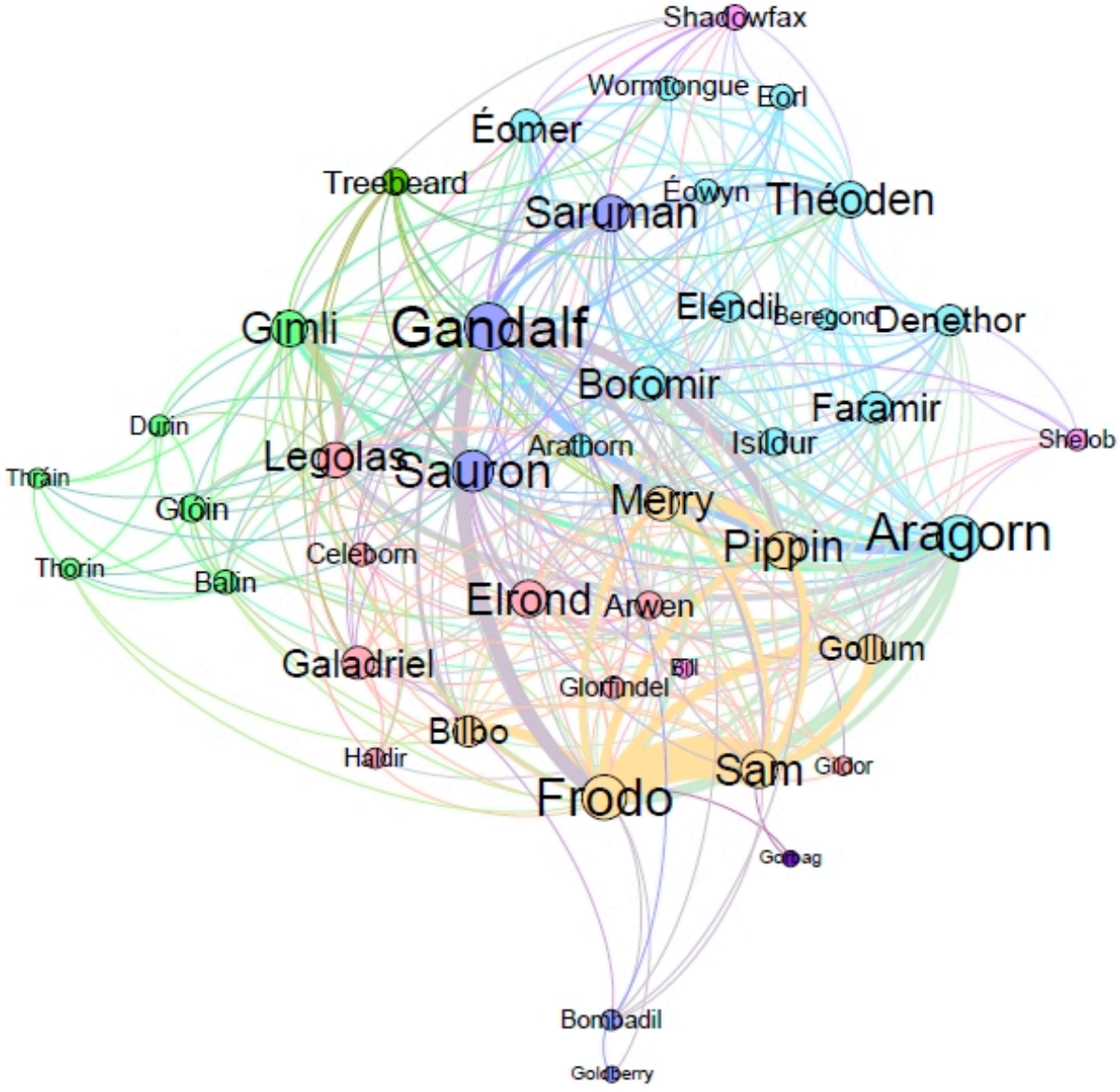
Example: Protein-Protein Interaction Network



What proteins are most important in the network?

Useful for analyzing mutations in diseases, drug development,...

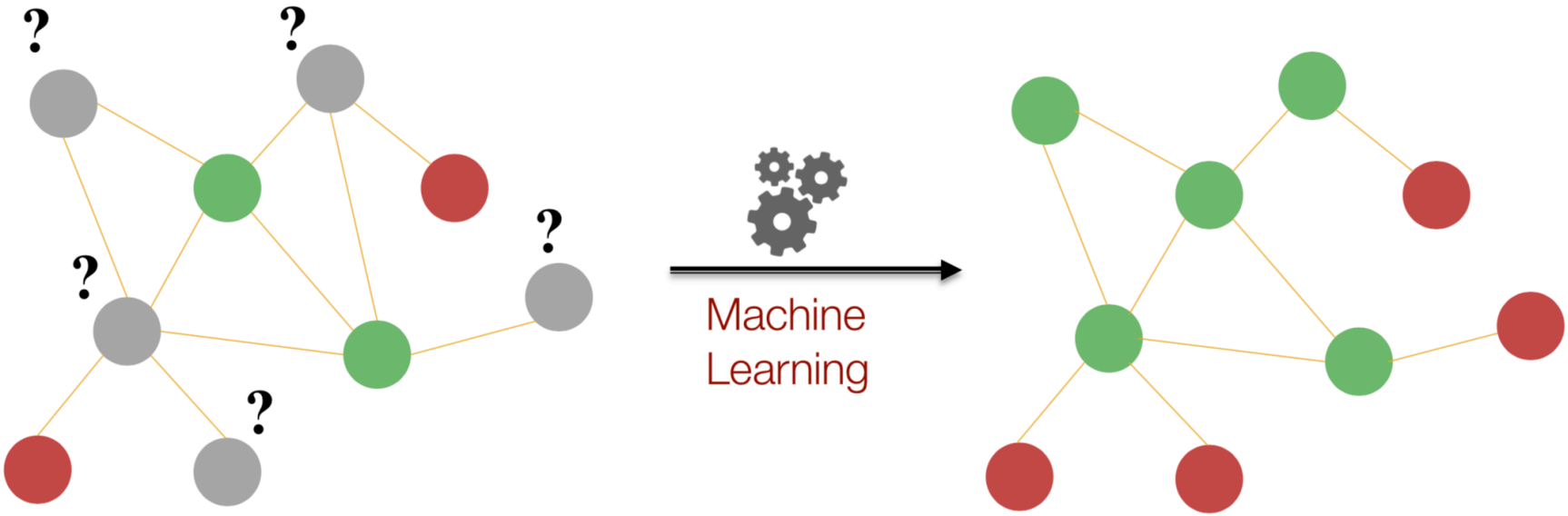
Motivation (continue)



http://www.morethanbooks.eu/graph-network-of-the-lord-of-the-rings/

Motivation: A Different View

If you have a machine learning task defined at the node level, you need *features* for nodes.



Features:

- *external*: qualities/measures for each node, not related to the network
- *topological*: features related to the network structure

The scores of importance are often good features for nodes.

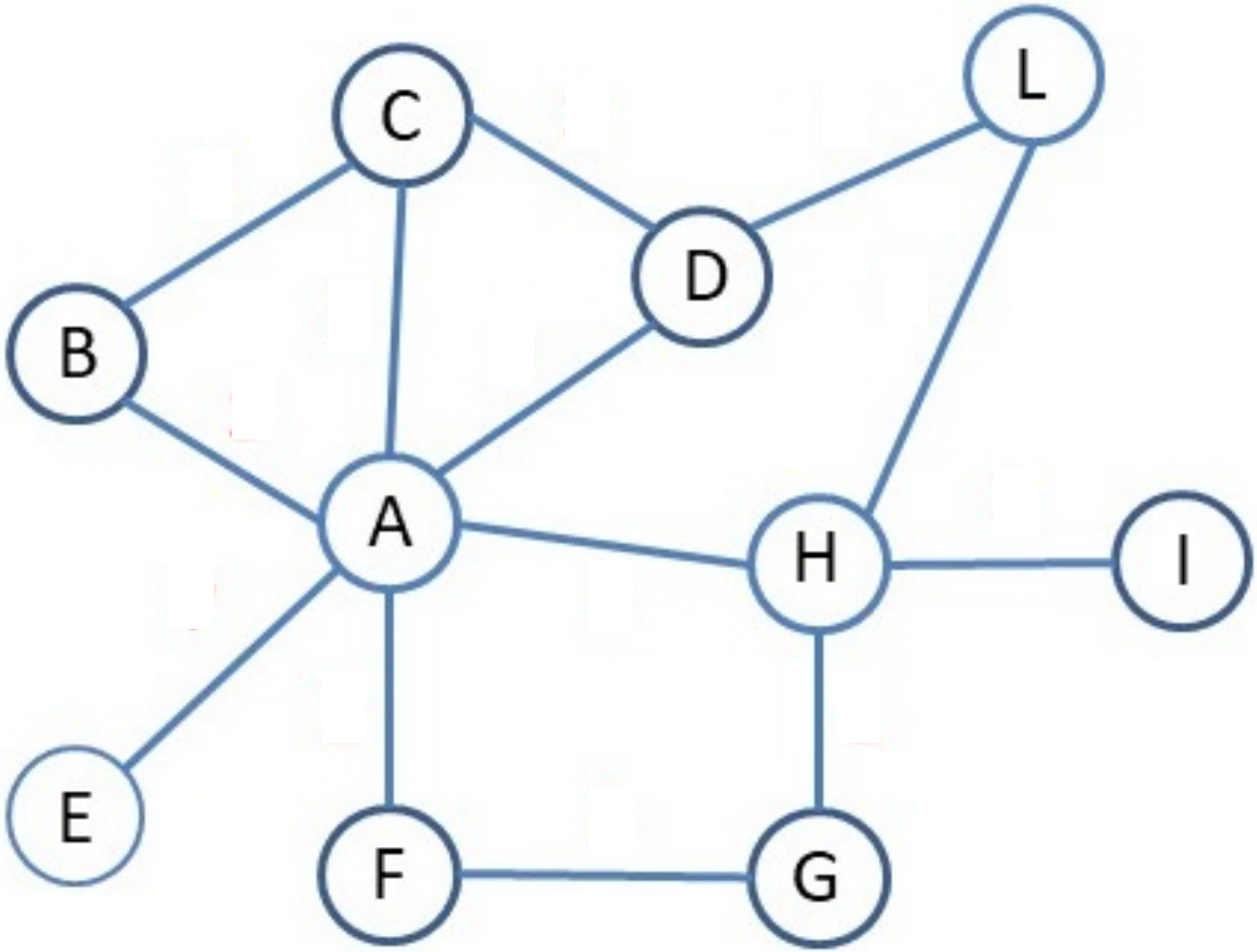
A First Score: Node Degree

What is the easiest node score we can derive from a network?

The **node degree**: $degree(u)$

Complexity to compute the node degree for all $v \in V$? $\mathcal{O}(|V|)$

Example



Node Centralities

Several scores have been proposed to measure the *centrality* of a node in a network.

The most important and commonly used ones are:

- *closeness* centrality
- *betweenness* centrality

Closeness Centrality

Intuition: a node is central if it is fairly *close* to the other nodes in the network.

Let $G = (V, E)$ be a connected, undirected graph (weighted or unweighted)

Definition

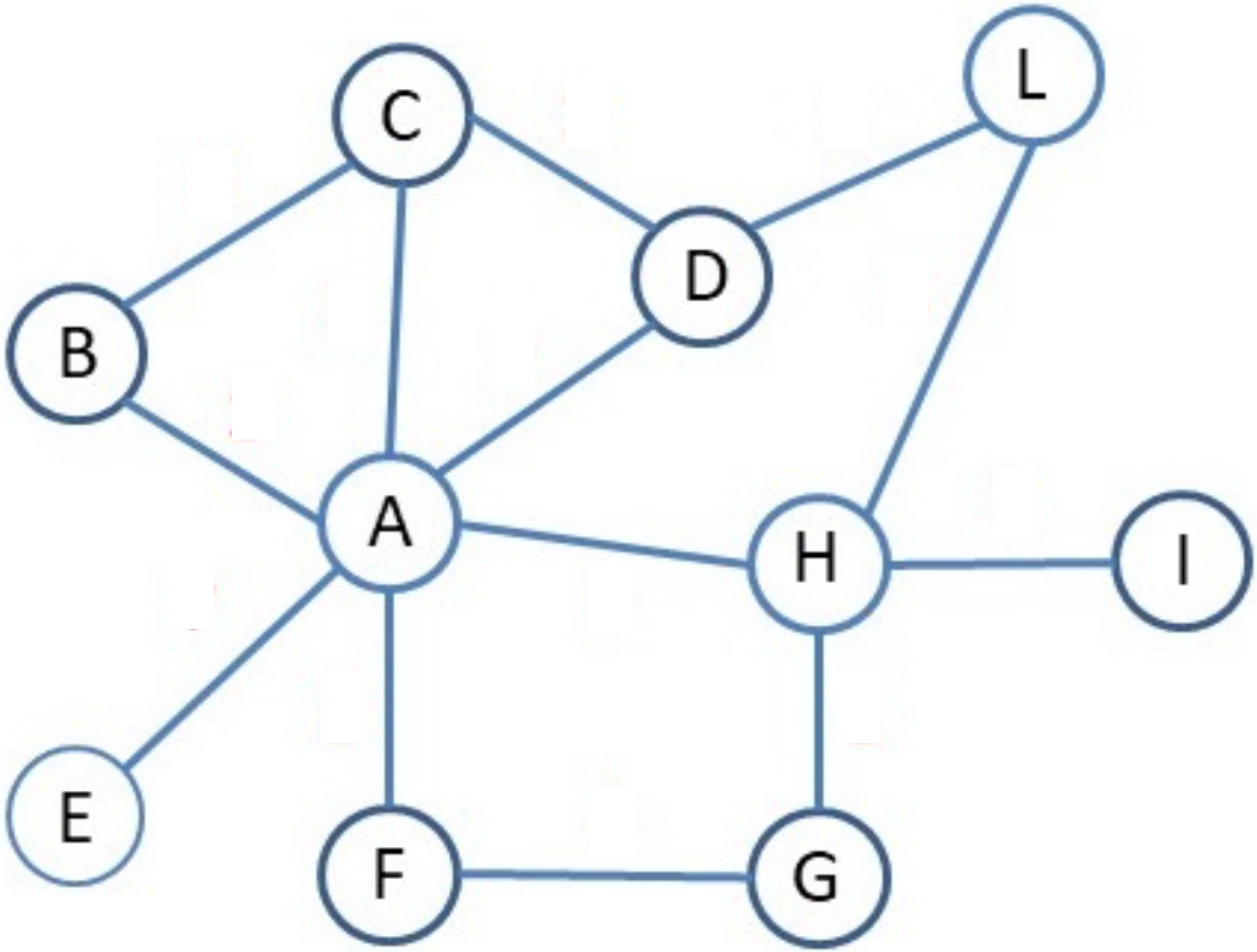
Given a node v, the closeness centrality $c(v)$ of v is:

$$c(v) = \frac{n-1}{\sum_{u \neq v, u \in V} d(v,u)}$$

Note: since $d(v,v) = 0$ for all $v \in V$:

$$c(v) = \frac{n-1}{\sum_{u \in V} d(v,u)}$$

Closeness Centrality: Example Unweighted Graph



Distance: Weighted vs Unweighted Graphs

Given $u, v \in V$, let $d(u, v)$ the *distance* between u and v.

G *unweighted*: $d(u, v)$ is the number of edges in a *shortest path* between u and v

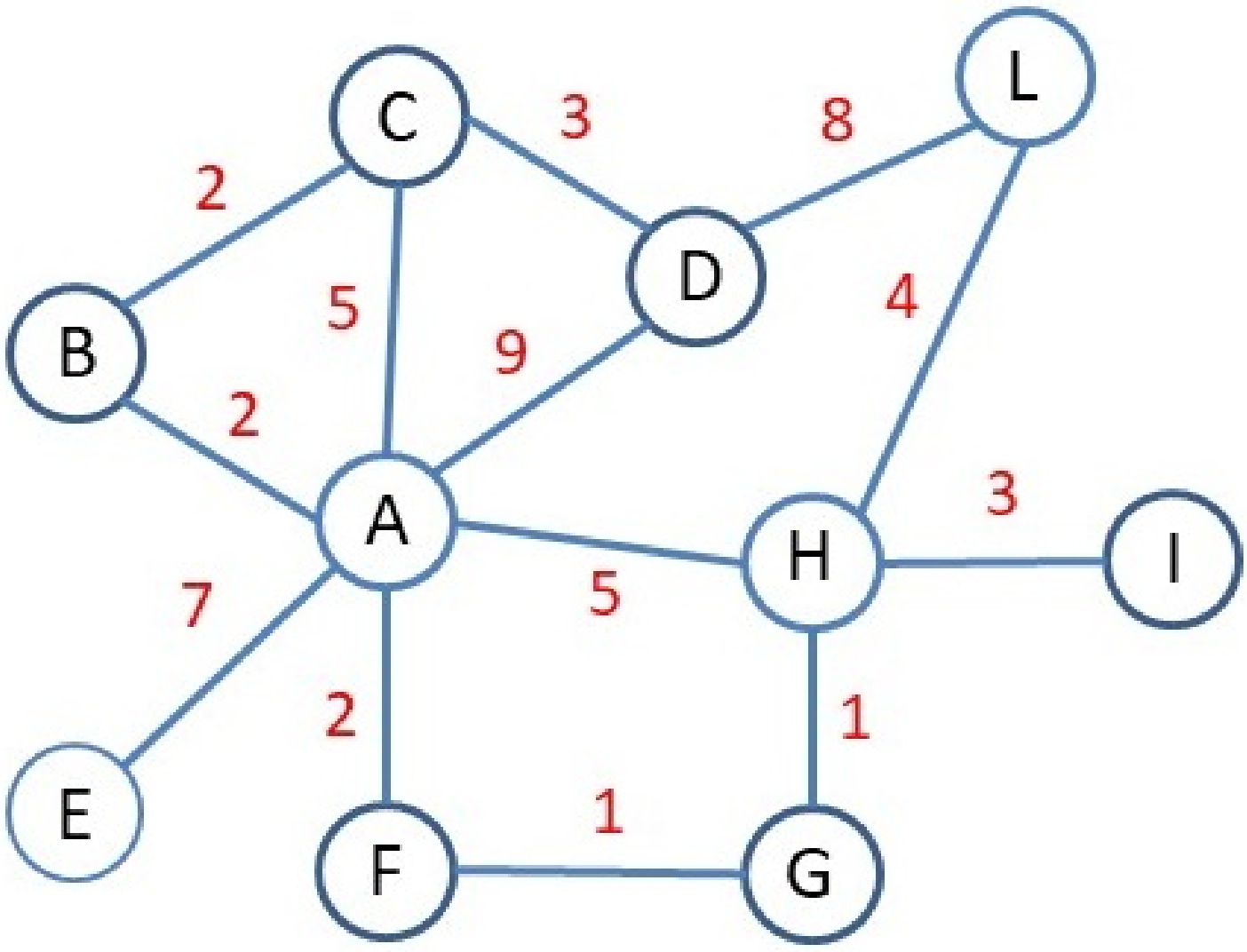
G *weighted*:

- edge weight function $w : E \to \mathbb{R}^+$ $(w(e) \in \mathbb{R}^+)$
- *length* of path $u_1, u_2, \ldots, u_k$ is:

$$\sum_{i=1}^{k-1} w(u_i, u_{i+1})$$

- $d(u, v)$ is the minimum length of a path from u to v
- a path of length $d(u, v)$ between u and v is a *shortest path*

Closeness Centrality: Example Weighted Graph



Computing Closeness Centrality: One Node

Given $v \in V$, how can we compute its closeness centrality $c(v)$?

We need the values $d(v, u)\ \forall u \in V$...

Definition

Given a simple, undirected graph $G = (V, E)$ and a vertex $v \in V$, the Single-Source Shortest Paths (SSSP) problem requires to find all the distances between v and the other vertices in V (and the relative shortest paths).

If G is unweighted: SSSP can be solved by a simple modification of $BFS(G, v)$!

Computing Closeness Centrality: One Node (continue)

Let $distBFS(G, v)$ be $BFS(G, v)$ with the following changes:

- every node $u \in V$ has a field $u.distance$
- initially: $u.distance$ has value $0, \forall u \in V$
- when node w is visited and then inserted in list L_{i+1}, we set $w.distance$ to $i + 1$. That is, the instruction

  "visit w"

  is substituted with

  "$w.distance \leftarrow i + 1$"

- complessità $\Theta(|E|)$ (grafo connesso)

Proposition

When $distBFS(G, v)$ terminates, $u.distance = d(v, u)$.

Computing Closeness Centrality: One Node (continue)

Algorithm `ClosenessCentrality`(G, v)
Input: unweighted graph $G = (V, E)$ with $|V| = n$ and $|E| = m$; $v \in V$
Output: closeness centrality c_v of v

`distBFS`(G, v); $\Theta(m)$
$sum_v \leftarrow 0$;
forall $u \in V$ **do**
  $sum_v \leftarrow sum_v + u.distance$; } $\Theta(n)$
return $(n-1)/sum_v$;

Complexity? $\Theta(n+m) = \Theta(m)$ dato che G connesso $\rightarrow m \geq n-1$

Computing Closeness Centralities

What about computing the node centralities of all nodes in G?

Algorithm `ClosenessCentralities`(G)
Input: unweighted graph $G = (V, E)$ with $|V| = n$ and $|E| = m$
Output: closeness centrality $c(v)$ for all $v \in V$
forall $v \in V$ **do**
  $c(v) \leftarrow$ `ClosenessCentrality`(G, v);
return values $c(v)$;

Complexity? $\Theta(n \cdot m) \Rightarrow$ dipende da relazione n, m

Computing Closeness Centrality: Weighted Graph

Let G be edge weighted: given $v \in V$, how can we compute its closeness centrality $c(v)$?

We need the values $d(v, u)\ \forall u \in V$...

Dijkstra algorithm: solves the SSSP problem using a *priority queue*

Complexity of Dijkstra algorithm: depends on how the *priority queue* is implemented

- priority queue implemented with a *heap*: $\Theta\left(\min\{n^2, (n+m)\log n\}\right)$
- priority queue implemented with a *Fibonacci heap* (list of heaps): $\Theta\left(m + n\log n\right)$

Computing Closeness Centralities: Weighted Graph

Let `ClosenessCentralityW`(G, v) be the algorithm, based on Dijkstra algorithm, to compute the closeness centrality for node v.

Analogously to before, the node centralities of all nodes in G are computed as follows. on Fibonacci heap: $O(m + n \log n)$

Algorithm `ClosenessCentralities`(G)
Input: weighted graph $G = (V, E, w)$ with $|V| = n$, $|E| = m$, $w : E \to \mathbb{R}^+$ connesso
Output: closeness centrality $c(v)$ for all $v \in V$

forall $v \in V$ **do**
  $c(v) \leftarrow$ `ClosenessCentralityW`(G, v);
return values $c(v)$;

Complexity? $\Theta(n(m + n \log n))$ if the version of Dijkstra algorithm based on Fibonacci heaps is used.

Can we do better?

Computing Closeness Centralities: Weighted Graph (continue)

We need the values $d(v, u)\ \forall u, v \in V$.

Definition

Given a simple graph $G = (V, E)$, the All-Pairs Shortest Paths (APSP) problem requires to find all the distances $d(u, v)$ for all pairs $u, v \in V$ (and the relative shortest paths).

Floyd-Warshall algorithm: solves the APSP!

meglio perché non sempre n^3

Complexity? $\Theta(n^3) \Rightarrow$ rispetto a $\Theta(n(m+n\log n))$, meglio se $m << n^2$

Johnson's algorithm: solves the APSP problem. Time? $\Theta(n^2 \log n + nm)$

Note: while these algorithms do not improve on Dijkstra algorithm, they can be used when negative weights are present (no negative-weight cycles are allowed).

Computing Closeness Centralities for Large Graphs

Up to know: we can compute the closeness centralities for all nodes in a network $G = (V, E)$, $|V| = n$, $|E| = m$, in time

- G unweighted: $\Theta(nm)$
- G weighted: $\Theta(n(m + n \log n))$

These complexities are impractical for large networks!

What about computing *approximations* of closeness centralities instead of the exact values?

Approximating Closeness Centralities

Any idea?

in calcolo c_v, uso solo
k distanze $d(v,u_1),\dots,d(v,u_k)$,
invece di tutte $(n-1)$
distanze $\Rightarrow$ stimo alla fine sarà

$$\hat{c}(v) = \frac{n-1}{\frac{n}{k}\sum_{i=1}^{k} d(v,u_i)}$$

$c(1) = d(1,1) + d(1,2) + \dots + d(1,n)$
$c(2) = d(2,1) + d(2,2) + \dots + d(2,n)$
$c(3) = d(3,1) + d(3,2) + \dots + d(3,n)$

$\Downarrow$

calcolo $c(1)$, poi posso riusare
$d(1,2)$ in $c(2)$

$\Downarrow$

anziché n BFS, calcolo k BFS

come scelgo k?

Approximating Closeness Centralities (continue)

Eppstein-Wang Algorithm

D. Eppstein, J. Wang, (2006). *Fast approximation of centrality.* Journal of Graph Algorithms and Applications, 5(5), 39.

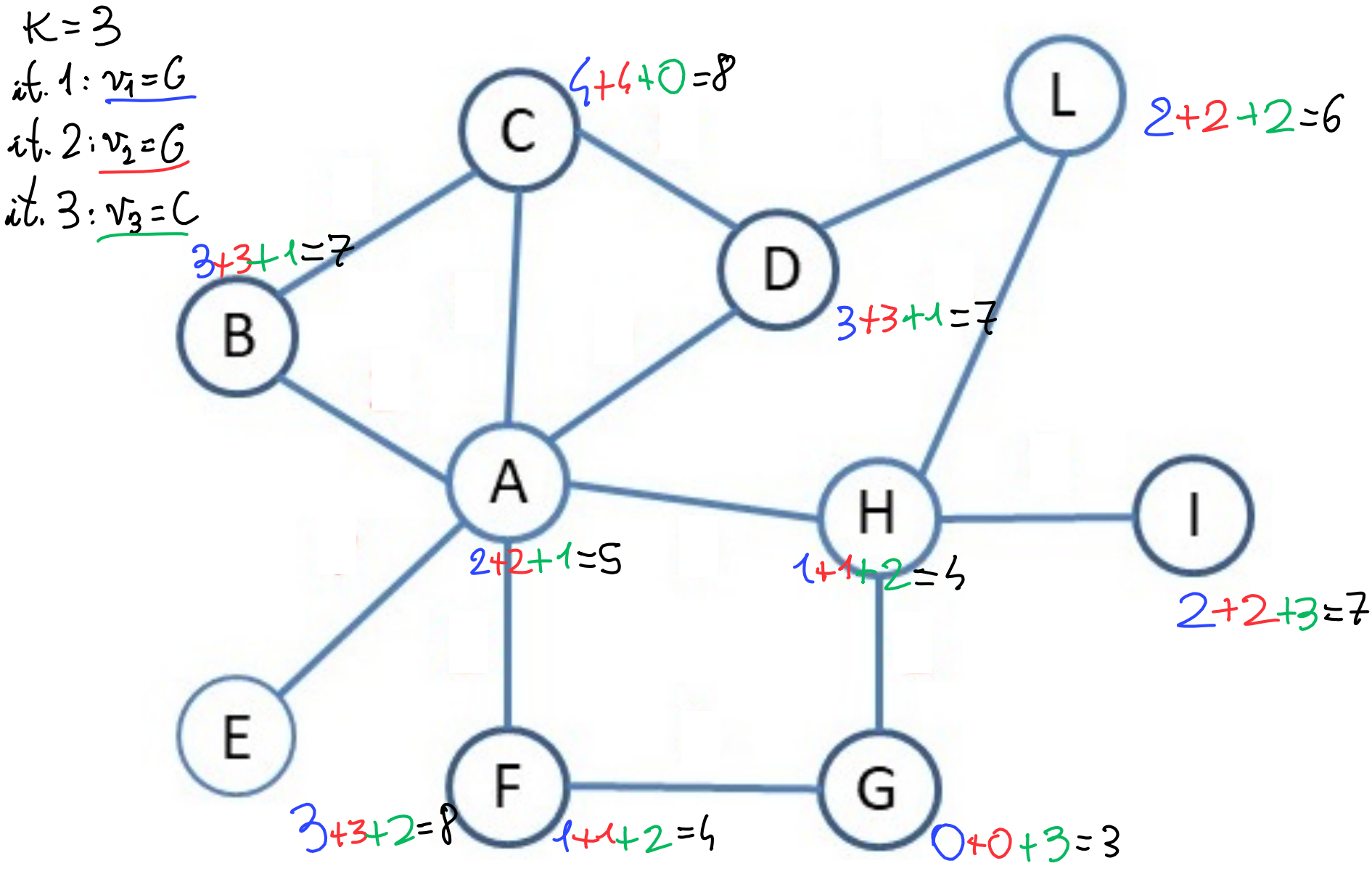
Same algorithm for both weighted and unweighted graphs, only difference: how the SSSP problem is solved.

Eppstein-Wang Algorithm (continue)

Algorithm `ApproximateClosenessCentralities`(G, k)
Input: weighted/unweighted graph $G = (V, E)$ with $|V| = n$, $|E| = m$; $k \in \mathbb{N}$ connesso
Output: approximation $\hat{c}(v)$ of $c(v)$ for all $v \in V$

$sum_v \leftarrow 0$ for all $v \in V$;
for $i \leftarrow 1$ *to* k **do**
    $v_i \leftarrow$ random vertex chosen uniformly at random from V;
    solve SSSP problem with source v_i;
    forall $v \in V$ **do**
        $sum_v \leftarrow sum_v + d(v_i, v)$;
forall $v \in V$ **do**
    $\hat{c}(v) \leftarrow 1/\left(\frac{n \cdot sum_v}{k(n-1)}\right)$;
return values $\hat{c}(v)$;

Eppstein-Wang Algorithm: Example



Eppstein-Wang Algorithm: Analysis

Ex: se $c(v)=0.49$ e $\hat{c}(v)=0.5$, $\left|\frac{1}{\hat{c}(v)}-\frac{1}{c(v)}\right| \approx 0.04$

// $=0.04$ // $=0.01$, // ≈ 15

For simplicity, we are going to consider the *inverse centrality estimator* $\frac{1}{\hat{c}(v)}$ and the *inverse centrality* $\frac{1}{c(v)}$.

Proposition

$$\mathbb{E}\left[\frac{1}{\hat{c}(v)}\right] = \frac{1}{c(v)}.$$

Dim: per certo v, X_i : r.v. con valore $d(v,v_i)\cdot\frac{n}{n-1}$, v_i = nodo scelto a it. i

$$\frac{1}{\hat{c}(v)} = \frac{1}{k}\cdot\sum_{i=1}^{k} X_i \Rightarrow \mathbb{E}\left[\frac{1}{\hat{c}(v)}\right] = \frac{1}{k}\cdot\sum_{i=1}^{k}\mathbb{E}[X_i]$$

in ogni it. i scegliamo v_i random uniformemente, ogni vertice ha prob. $\frac{1}{n}$ di essere scelto $\Rightarrow \forall i\in[1,k]$, $\mathbb{E}[X_i] = \sum_{j=1}^{n}\frac{1}{n}\cdot d(v,v_j)\cdot\frac{n}{n-1} =$

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

$$\mathbb{E}\left[\frac{1}{\hat{c}(v)}\right] = \frac{1}{k} \cdot \sum_{i=1}^{k} \frac{1}{n-1} \left(\sum_{u \in V} d(v,u) \right) = \frac{1}{k} \cdot \frac{k}{n-1} \cdot \sum_{u \in V} d(v,u) =$$

$$= \frac{1}{n-1} \sum_{u \in V} d(v,u) = \frac{1}{c(v)} \quad \blacksquare$$

Eppstein-Wang Algorithm: Analysis (continue)

We are now going to prove that the estimates $\frac{1}{\hat{c}(v)}$ are close to their expectations $\frac{1}{c(v)}$ if the number k of iterations in the algorithm is *large enough*.

We use (without proving it) the following *concentration* result.

Hoeffding's inequality

Let $X_1, X_2, \ldots, X_k$ are independent random variables, with $a_i \leq X_i \leq b_i$ for all $i \in \{1, \ldots, k\}$ and let $\mu = \mathbb{E}\left[\frac{\sum_{i=1}^{k} X_i}{k}\right]$.
Then for $\varepsilon > 0$:

$$\mathbb{P}\left[\left|\frac{\sum_{i=1}^{k} X_i}{k} - \mu\right| \geq \varepsilon\right] \leq 2e^{-2k^2\varepsilon^2 / \sum_{i=1}^{k}(b_i - a_i)^2}$$

Eppstein-Wang Algorithm: Analysis (continue)

Let $\Delta(G) = \max_{u,v \in V} d(u,v)$ be the *diameter* of a graph G.

Proposition

Let $\varepsilon > 0$ and $\delta \in (0,1)$ be constants. If $k \geq \frac{1}{2\varepsilon^2}\left(\log \frac{2n}{\delta}\right)\left(\frac{n}{n-1}\right)^2$ then the inverse centrality estimator $1/\hat{c}(v)$ from `ApproximateClosenessCentralities`(G,k) is within an additive factor $\varepsilon\Delta(G)$ of $1/c(v)$ *for all vertices* $v \in V$ with probability $\geq 1-\delta$.

Note: in several real-world networks $\Delta(G) \in O(\log n)$ - *small world phenomenon*.

Eppstein-Wang Algorithm: Analysis (continue)

Corollary

If $k \in \Theta\left(\frac{\log n}{\varepsilon^2}\right)$ for a constant $\varepsilon > 0$, then the inverse centrality estimator $1/\hat{c}(v)$ from `ApproximateClosenessCentralities`(G, k) is within an additive factor $\varepsilon\Delta(G)$ of $1/c(v)$ *for all vertices* $v \in V$ *with high probability*, i.e. with probability $\geq 1 - 1/n$.

Eppstein-Wang Algorithm: Complexity

The solution of k SSSP problems are needed.

- G unweighted: $\Theta(km)$
- G weighted: $\Theta(k(m + n \log n))$

Fixing $k \in \Theta\left(\frac{\log n}{\varepsilon^2}\right)$ as in the Corollary, the complexity is:

- G unweighted: $\Theta\left(\frac{m \log n}{\varepsilon^2}\right)$
- G weighted: $\Theta\left(\frac{\log n}{\varepsilon^2}(m + n \log n)\right)$

Closeness Centrality: More Advanced Algorithms

While Eppstein-Wang algorithm provides rigorous guarantees and useful results, the error of the estimates may be large when the distribution of distances in G is skewed (e.g., the diameter $\Delta(G)$ is large).

More advanced algorithm to estimate closeness centralities:
S. Chechik, E. Cohen, and H. Kaplan. *Average distance queries through weighted samples in graphs and metric spaces: high scalability with tight statistical guarantees.* APPROX/RANDOM 2015.

Closeness Centrality: Chechik-Cohen-Kaplan algorithm

Basic idea: use sampling to choose a sample S of k nodes for which the SSSP problem is solved and use the corresponding distances to estimate centralities for all nodes (as in Eppstein-Wang algorithm).

Main difference with Eppstein-Wang: S is not picked by choosing nodes uniformly at random

- for each vertex $v \in V$, compute a probability p_v, then include v in S with probability p_v independently of all other events (*Poisson sampling*)
- p_v's computation:
  - first draw a small sample S_0 (uniformly at random) and compute $W_s = \sum_{v \in V} d(s, v)$ for all $s \in S_0$
  - $p_v = \max\left\{\frac{1}{n}, \max_{s \in S_0} \frac{d(s,v)}{W_s}\right\}$

Provides better guarantees than Eppstein-Wang (e.g., no dependence on the diameter $\Delta(G)$ of G).

Closeness Centrality: Example

Bergamini et al., 2019. *Computing top-k Closeness Centrality Faster in Unweighted Graphs*, ACM Transactions on Knowledge Discovery from Data (TKDD).

Analysis of the Internet Movie DataBase (IMDB) graph:

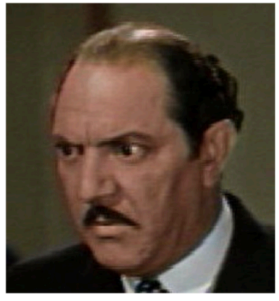
- nodes are actors;
- edges: two actors are connected if they played together in a movie (TV-series are ignored)

Considered:

- *snapshots* of the actor graph, taken every 5 years from 1940 to 2010, and 2014.
- some genres excluded: awards shows, documentaries, game-shows, news, realities, and talk-shows

Closeness Centrality: Example (continue)

Most central actors in the IMDB graph with respect to the closeness centrality measure.

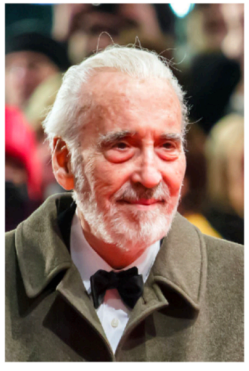


Semels ('40)

Corrado ('45)

Flowers ('50-'80)

Welles ('85-'90)



Lee ('95-'00)

Hitler ('05-'10)

Madsen ('14)

Top 10

2014
Madsen, Michael (I)
Trejo, Danny
Hitler, Adolf
Roberts, Eric (I)
De Niro, Robert
Dafoe, Willem
Jackson, Samuel L.
Keitel, Harvey (I)
Carradine, David
Lee, Christopher (I)

Closeness Centrality for Disconnected Graphs?

Various extension's, we consider: *Lin's index* [N. Lin. Foundations of social research. McGraw-Hill, 1976.]

Let $G = (V, E)$ be an undirected graph. Let C_v be the size of the connected component of v, i.e., of the set of vertices reachable from v. Let $n_v = |C_v|$.

Definition

Lin's index for $v \in V$ is

$$c(v) = \frac{(n_v - 1)^2}{(n-1)\sum_{u \in C_v} d(v,u)}$$

Note that

$$c(v) = \frac{(n_v - 1)^2}{(n-1)\sum_{u \in C_v} d(v,u)} = \frac{n_v - 1}{\sum_{u \in C_v} d(v,u)} \frac{n_v - 1}{n-1}$$

Betweenness Centrality

Intuition: a node is central if it *appears on several shortest paths* in the network.

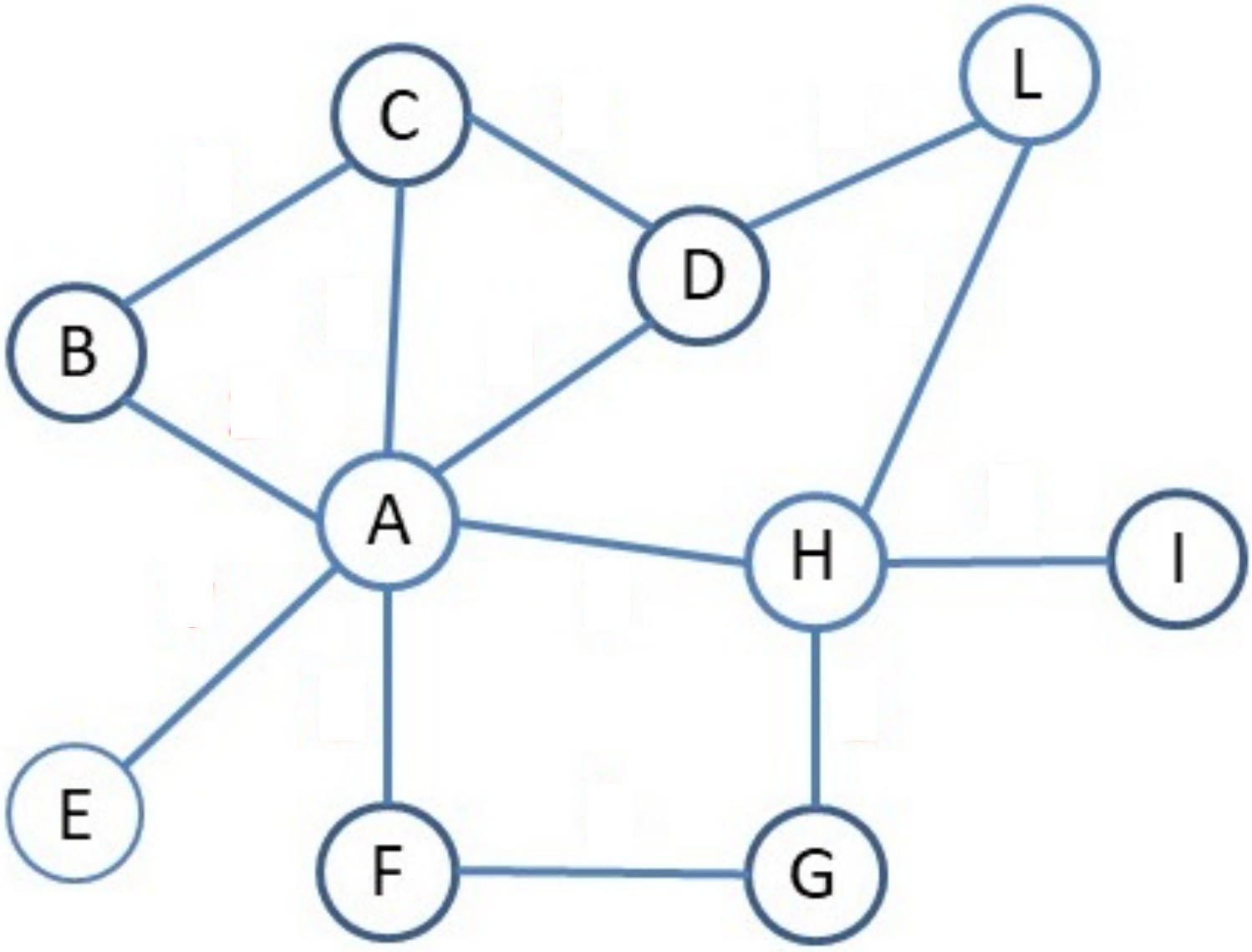
Let $G = (V, E)$ be an undirected graph (weighted or unweighted) with $|V| = n$
Let $\sigma_{s,t}$ be the number of shortest paths from node s to node t
Let $\sigma_{s,t}(v)$ be the number of shortest paths from node s to node t that pass through node v.

Definition

Given a node v, the betweennes centrality $b(v)$ of v is:

$$b(v) = \sum_{s,t \in V : s \neq v \neq t} \frac{\sigma_{s,t}(v)}{\sigma_{s,t}}$$

Betweenness Centrality: Example



Betweenness Centrality (continue)

Note: from the previous definition $b(v)$ can be > 1.

Definition

Given a node v, the normalized betweennes centrality $b(v)$ of v is:

$$b(v) = \frac{1}{n(n-1)} \sum_{s,t \in V : s \neq v \neq t} \frac{\sigma_{s,t}(v)}{\sigma_{s,t}}$$

Note: given G, $n = |V|$ is fixed $\Rightarrow$ the two definitions are equivalent.

Computing the Betweenness Centrality

To compute $b(v)$, we need to compute for each $s, t \in V$ ($s \neq v \neq t$):

- $\sigma_{s,t}(v)$
- $\sigma_{s,t}$

How? Brandes's algorithm [Brandes (2001). *A faster algorithm for betweenness centrality*. Journal of Mathematical Sociology.]

Idea: use a *augmented BFS*, which works also for weighted graphs

Complexity:

- G is unweighted: $O(nm)$
- G is weighted: $O(n(m + n \log n))$

Unfeasable for large graphs!

Approximating Betweenness Centralities

Algorithm `ApproximateBetweennessCentralities`(G, k)
Input: weighted/unweighted graph $G = (V, E)$ with $|V| = n$, $|E| = m$; $k \in \mathbb{N}$
Output: approximation $\hat{b}(v)$ of $b(v)$ for all $v \in V$

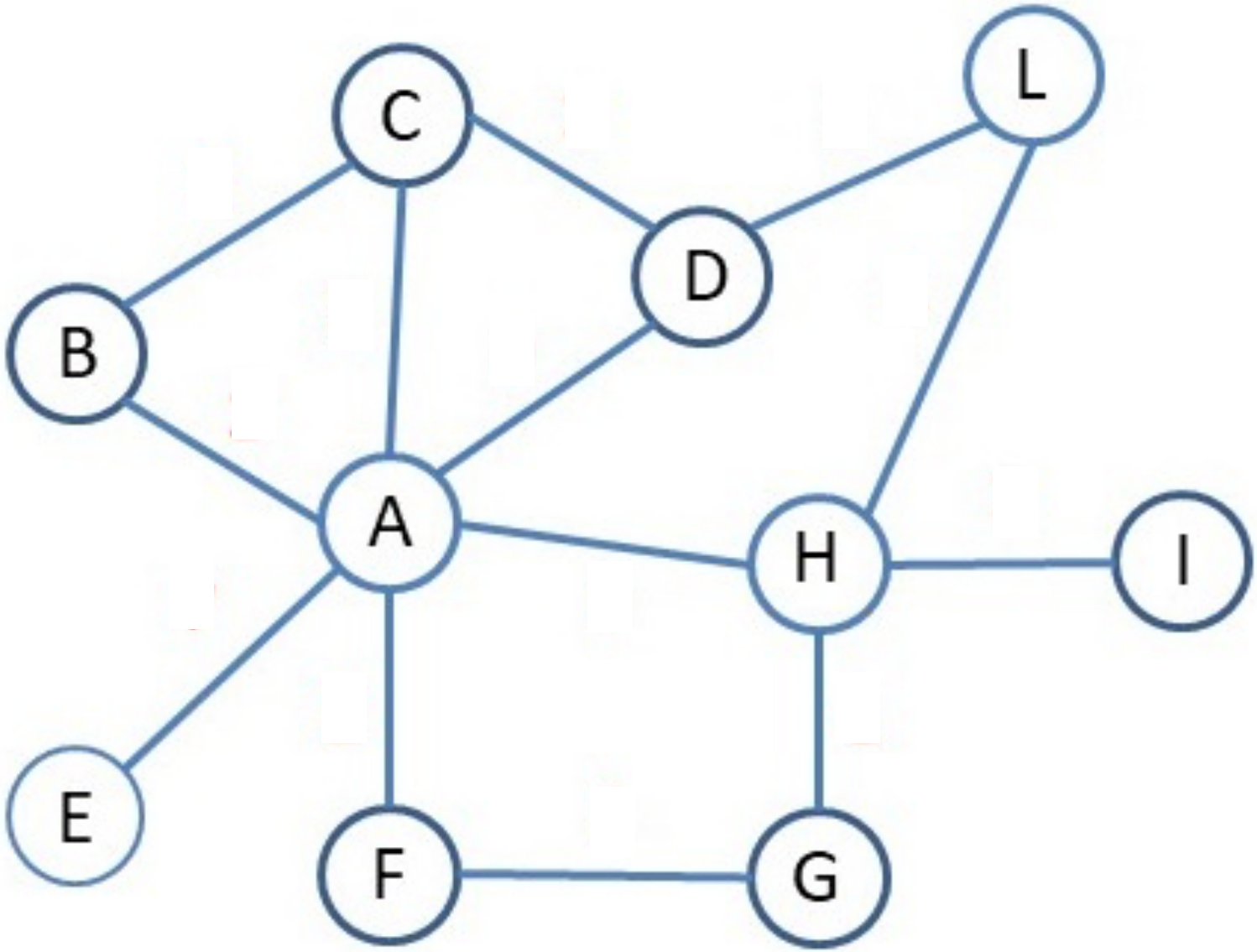
$\hat{b}(v) \leftarrow 0$ for all $v \in V$;
for $i \leftarrow 1$ *to* k **do**
    $(s, t) \leftarrow$ uniform vertex pair from V with $s \neq t$;
    $\mathcal{P}_{s,t} \leftarrow$ all shortest paths from s to t;
    $\pi_i \leftarrow$ shortest path chosen uniformly at random from $\mathcal{P}_{s,t}$;
    forall $v \in \pi_i$ **do**
        if $v \neq s$ *and* $v \neq t$ **then** $\hat{b}(v) \leftarrow \hat{b}(v) + \frac{1}{k}$;
return values $\hat{b}(v)$;

Approximating Betweenness Centralities (continue)

Note:

- $\mathcal{P}_{s,t}$ can be computed by a modified SSSP algorithm (BFS for unweighted graphs, Dijkstra's algorithm for weighted graphs) that keeps track of *all shortest paths*
- the SSSP algorithm starts from s and can stop as soon as all shortest paths to t are found

Approximating the Betweenness Centrality: Example



Approximating the Betweenness Centrality: Analysis

Proposition

For any $v \in V$:

$$\mathbb{E}\left[\hat{b}(v)\right] = b(v)$$

Approximating the Betweenness Centrality: Analysis (continue)

How many samples are needed to have $\hat{b}(v)$ close to $b(v)$?

vertex diameter $VD(G)$ of G: maximum number of vertices among all shortest paths in G. ($VD(G) - 1$ is equal to the *diameter* of G if G is unweighted.)

Riondato, Karnaropoulos (2016)

If $k \geq \frac{2}{\varepsilon^2}\left(\lfloor \log_2(VD(G) - 2) \rfloor + \ln(1/\delta)\right)$, then

$$\Pr[\exists v \in V s.t. |\hat{b}(v) - b(v)| > \varepsilon] < \delta.$$

Proof: based on the VC dimension of shortest paths.

Other improvements: Riondato and Upfal (2018), Borassi and Natale (2019), Pellegrina and Vandin (2023).

Other Centrality Measures

There are several other centrality measures often implemented in graph analytics libraries:

- PageRank centrality
- harmonic centrality
- ...

Some useful libraries:

- https://graph-tool.skewed.de/
- https://networkx.org/
- https://networkit.github.io/
- https://snap.stanford.edu/

Comparison on Zachary's Karate Club Data

See jupyter notebook.