

# Similarities

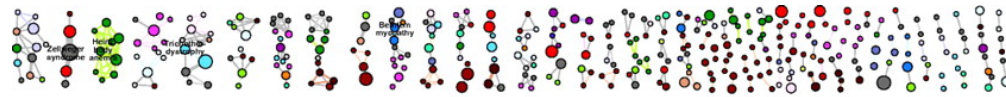
Why do we need to compute them?

For example, imagine a simple movie database with three sets of elements (or tables), `people`, `movie`, and `movie_category`, and two relationships `has_watched`, between `people` and `movie`, and `belongs_to`, between `movie` and `movie_category`.

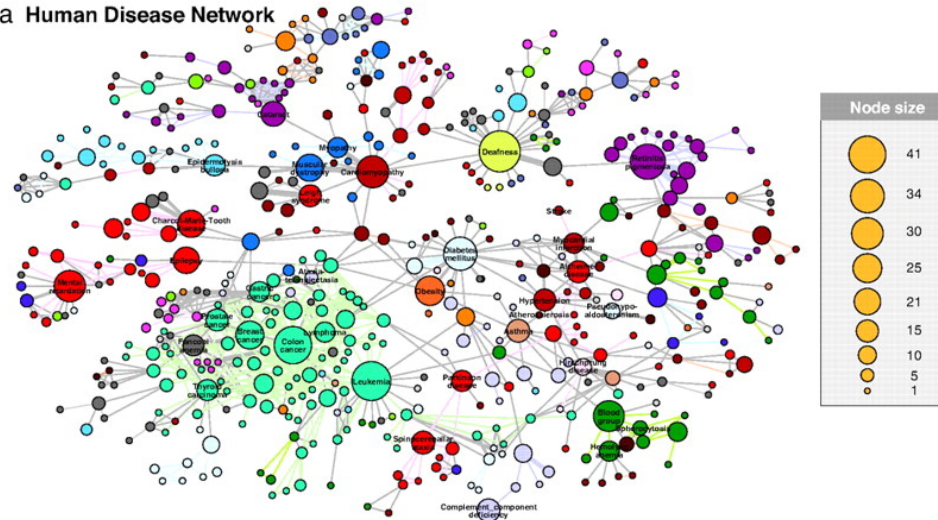
- Computing similarities between people allows us to cluster them into groups with similar interest about watched movies.
- Computing similarities between people and movies allows us to suggest movies to watch or not to watch.
- Computing similarities between people and movie categories allows us to attach a most relevant category to each person.

[FPRS] Random-walk based similarities

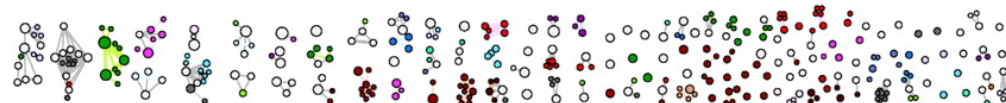
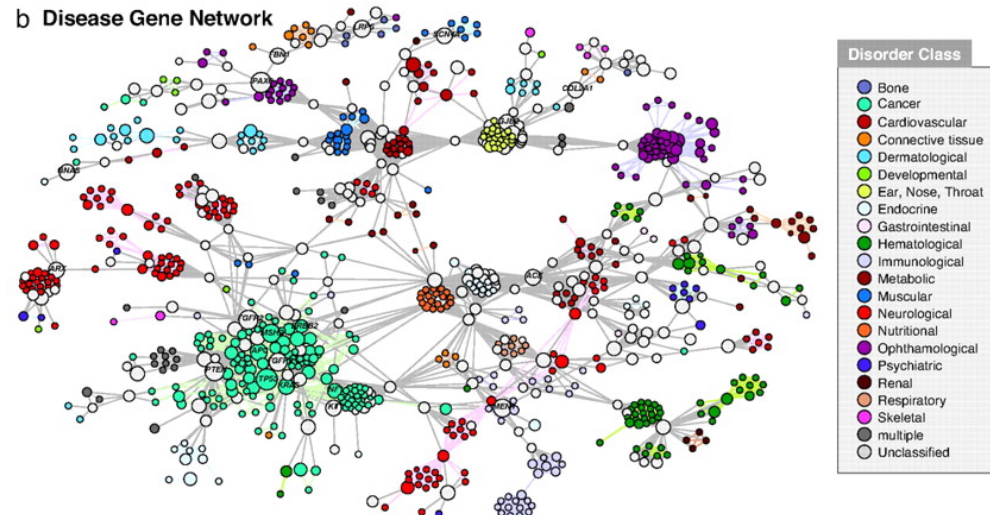
# Similarities



a Human Disease Network



b Disease Gene Network



Goh et al. "Human Disease Network",  
PNAS, 2007

# Classes of Similarities

Q: In what ways can vertices in a network be similar and how can we quantify this similarity?

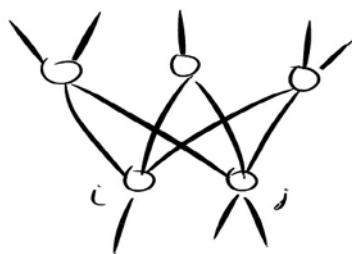
Similarity between vertices

Structural equivalence

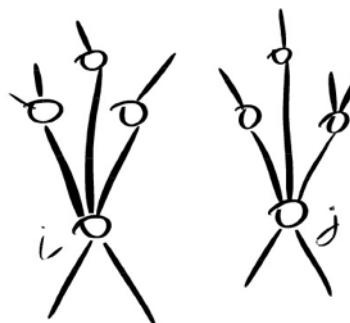
Regular equivalence

$i$  and  $j$  share many of the same network neighbors

$i$  and  $j$  do not necessarily share neighbors but have neighbors who are themselves similar



Structural



Regular

# Structural Equivalence

- Number of common neighbors, i.e.,  $n_{ij} = \sum_k A_{ik}A_{kj} = ij$ th element of  $A^2$
- Cosine similarity

$$\sigma_{ij} = \cos \theta = \frac{\sum_k A_{ik}A_{kj}}{\sqrt{\sum_k A_{ik}^2} \sqrt{\sum_k A_{kj}^2}} = \frac{n_{ij}}{\sqrt{d(i)d(j)}} \in [0, 1]$$

$$\langle A_i \rangle = \frac{1}{n} \sum_k A_{ik}$$

- Pearson coefficients

$$\begin{aligned} \sum_k A_{ik}A_{jk} - \frac{d(i)d(j)}{n} &= \sum_k A_{ik}A_{jk} - \frac{1}{n} \sum_k A_{ik} \sum_l A_{jl} \\ &= \sum_k A_{ik}A_{jk} - n \langle A_i \rangle \langle A_j \rangle = \sum_k [A_{ik}A_{jk} - \langle A_i \rangle \langle A_j \rangle] \end{aligned}$$

$\approx$ expected number of common neighbors

$$= \sum_k (A_{ik} - \langle A_i \rangle)(A_{jk} - \langle A_j \rangle) = n \cdot \text{cov}(A_i, A_j)$$

$$r_{ij} = \frac{\text{cov}(A_i, A_j)}{\sigma_i \sigma_j} = \frac{\sum_k (A_{ik} - \langle A_i \rangle)(A_{jk} - \langle A_j \rangle)}{\sqrt{\sum_k (A_{ik} - \langle A_i \rangle)^2} \sqrt{\sum_k (A_{jk} - \langle A_j \rangle)^2}}, \quad -1 \leq r_{ij} \leq 1$$

- Euclidean distance (number of neighbors that differ)  $d_{ij} = \sum_k (A_{ik} - A_{jk})^2$

# Regular Equivalence

The vertices have neighbors that are themselves similar

$$\sigma = \alpha A \sigma A \text{ or } \sigma_{ij} = \alpha \sum_{kl} A_{ik} A_{jl} \sigma_{kl} \leftarrow \text{similarity}$$

Problem:  $\sigma_{ii}$  is not necessarily high

Solution: extra diagonal term

$$\sigma = \alpha A \sigma A + I \text{ or } \sigma_{ij} = \alpha \sum_{kl} A_{ik} A_{jl} \sigma_{kl} + \zeta_{ij}$$

Still problem: in iterative calculation (init 0) we count only even paths

**New formulation:**  $i$  and  $j$  are similar if  $i$  has a neighbor  $k$  that is similar to  $j$

$$\sigma = \alpha A \sigma + I \text{ or } \sigma_{ij} = \alpha \sum_k A_{ik} \sigma_{kj} + \zeta_{ij}$$

Convergence:  $\sigma = \sum_{m=0}^{\infty} (\alpha A)^m = (I - \alpha A)^{-1}$

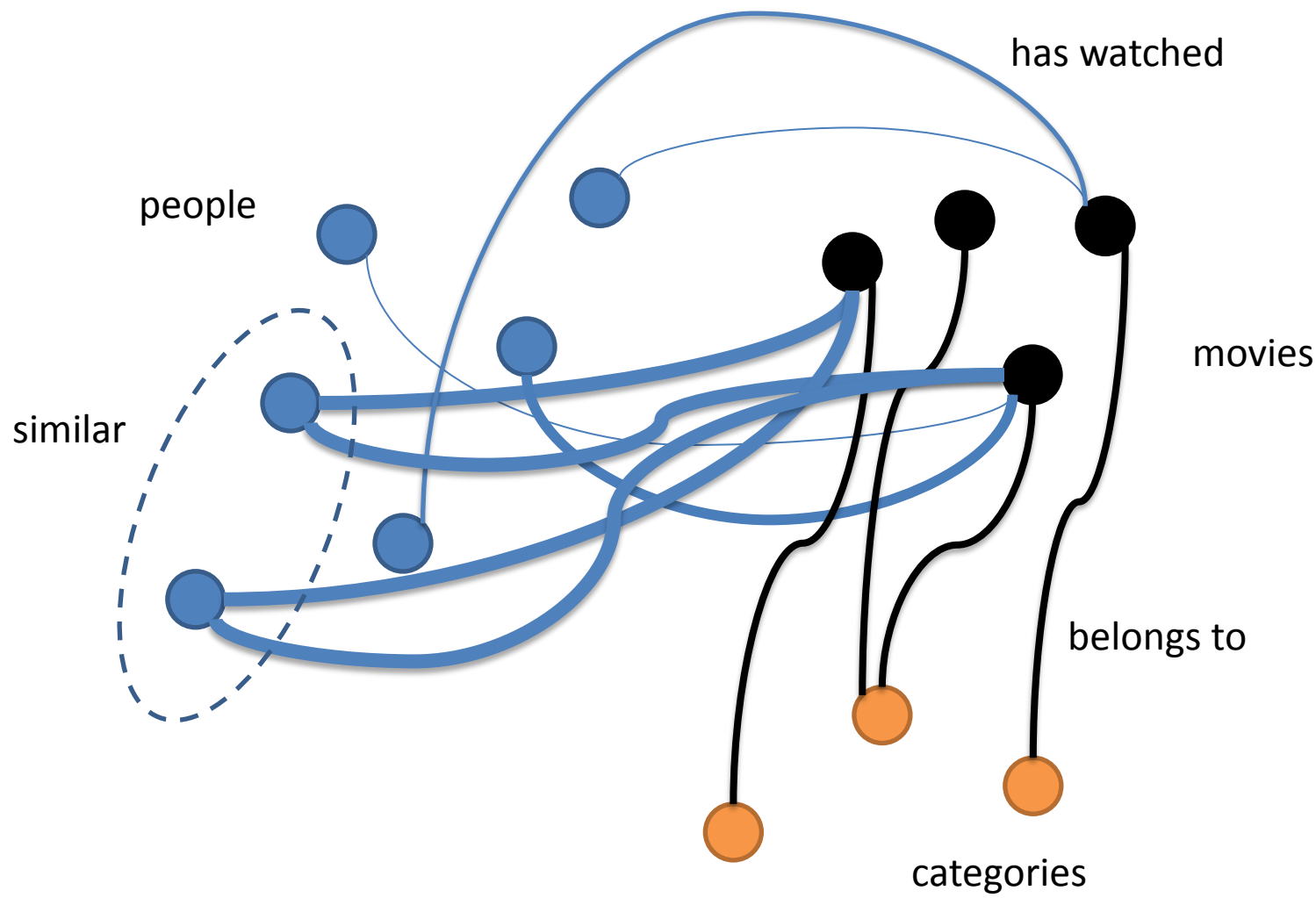
Another problem: too high similarity for high-degree nodes which is not necessarily true

Solution: divide by  $d(i)$

$$\sigma = \alpha D^{-1} A \sigma + I \text{ or } \sigma_{ij} = \frac{\alpha}{d(i)} \sum_k A_{ik} \sigma_{kj} + \zeta_{ij}$$

 PDF: Algebraic Distance

# Random walk based similarities



[FPRS] Random-walk based similarities

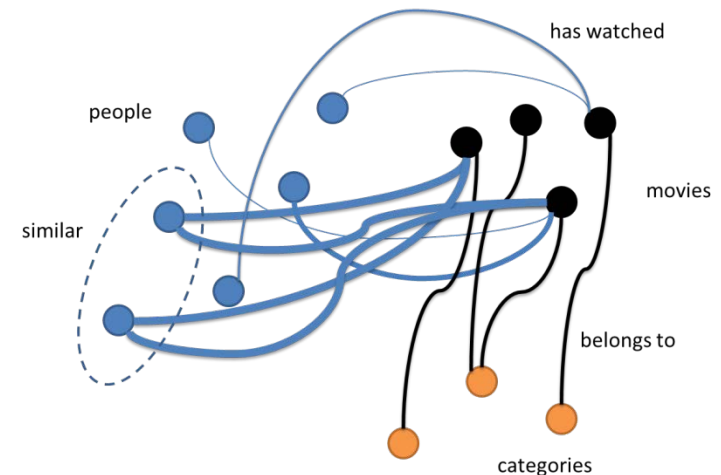
# Random walk based similarities

The Markov chain ( $t$  - step,  $s(t)$  - state at  $t$ ) describing the sequence of nodes visited by a random walker is called a random walk. The random walk is defined with the following single-step transition probabilities of jumping from any state or node  $i = s(t)$  to an adjacent node

$$j = s(t + 1) : Pr(s(t + 1) = j | s(t) = i) = a_{ij} / a_{ii} = p_{ij},$$

where  $a_{ii} = \sum_{j=1}^n a_{ij}$ . The probability of being in state  $i$  at time  $t$  is  $\pi_i(t) = Pr(s(t) = i)$  and  $P$  is the transition matrix with entries  $p_{ij}$ . The evolution of Markov chain is given by

$$\pi(t + 1) = P^T \pi(t)$$



[FPRS] Random-walk based similarities



# Random walk based similarities

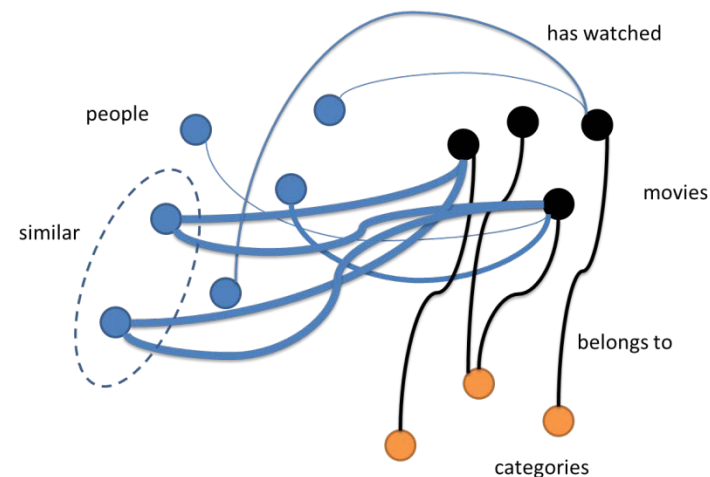
The average first-passage time  $m(k|i)$  is the average number of steps that a random walker, starting in (random) state  $i \neq k$ , will take to enter state  $k$  for the first time, i.e.,

$$m(k|i) = E[T_{ik} | s(0) = i], \text{ where } T_{ik} = \min(t \geq 0 | s(t) = k, s(0) = i).$$

The average first-passage cost  $o(k|i)$  is the average cost incurred by the random walker starting from state  $i$  to reach state  $k$  for the first time. The cost of each transition is given by  $c(j|i)$ .

$$\begin{cases} m(k|k) = 0 \\ m(k|i) = 1 + \sum_{j=1}^n p_{ij} m(k|j), \text{ for } i \neq k, \end{cases}$$

$$\begin{cases} o(k|k) = 0 \\ o(k|i) = \sum_{j=1}^n p_{ij} c(j|i) + \sum_{j=1}^n p_{ij} o(k|j), \text{ for } i \neq k. \end{cases}$$

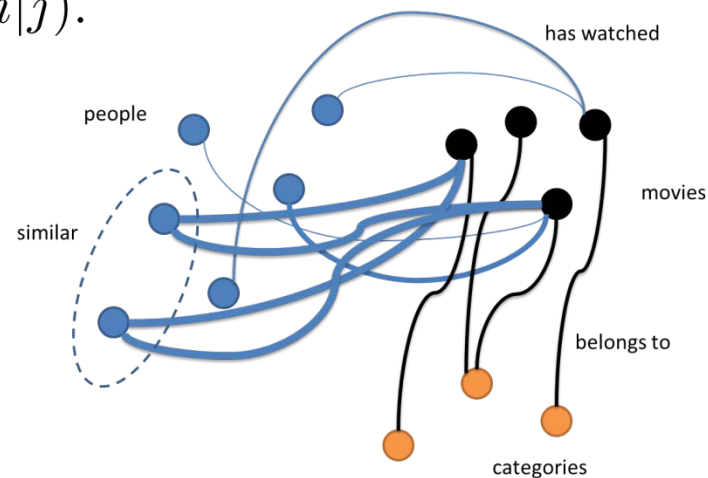


[FPRS] Random-walk based similarities

# Random walk based similarities

The average commute time  $n(i, j)$  is the average number of steps that a random walker, starting in state  $i \neq j$ , will take to enter state  $j$  for the first time and go back to  $i$ , i.e.,

$$n(i, j) = m(j|i) + m(i|j).$$



Homework: review of “Random-Walk Computation of Similarities between Nodes of a Graph with Application to Collaborative Recommendation”  
Submit by 2/11/2014

[FPRS] Random-walk based similarities