Graph similarity algorithms

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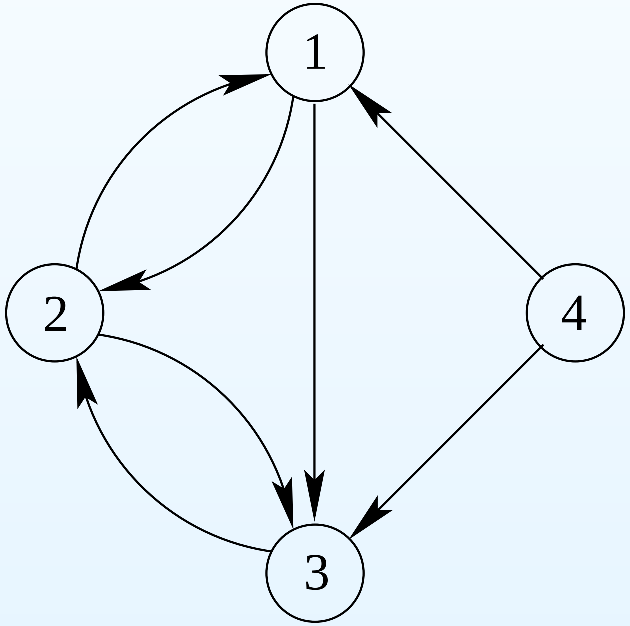
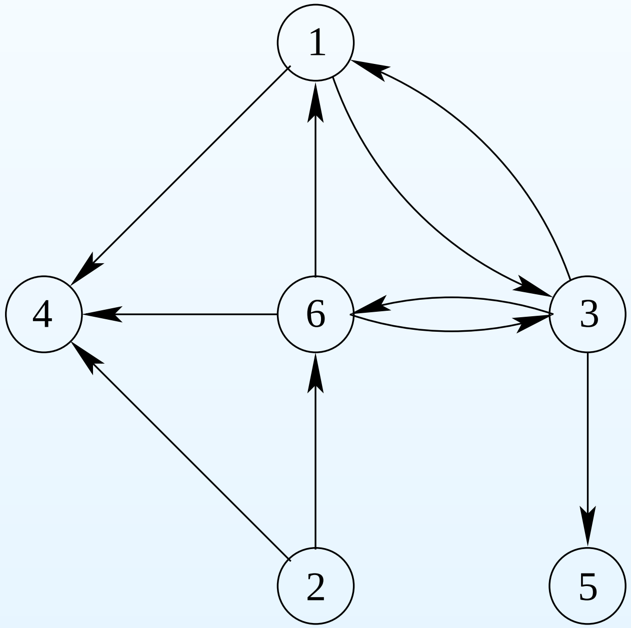
Similarity scores between nodes of graphs

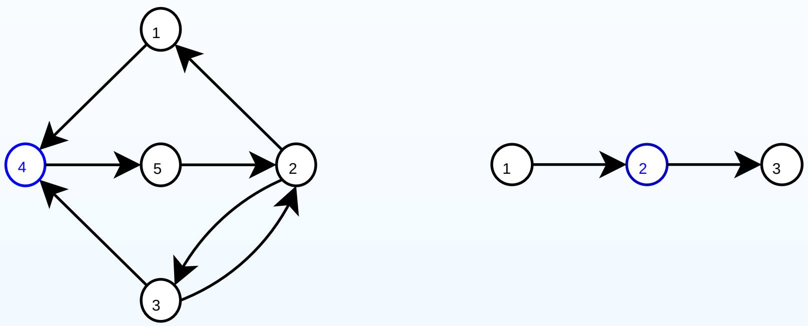
How can we compare the nodes of two graphs?





Similarity of nodes

Two nodes will be similar if they have similar in/out neighbors



- Similarity score between 4 of G_A and 2 of G_B:

$$s(a_4, b_2) \leftarrow s(a_1, b_1) + s(a_3, b_1) + s(a_5, b_3).$$

- Simultaneous iterative computation of the scores of all the pairs.
- The score of a pair is reinforced by the scores of its “neighbors pairs”.

[Blondel, Gajardo, Heymans, Senellart, Van Dooren 2004]
[Melnik,Garcia-Molina,Rahm 2002]

Computation of the similarity scores

- Let A and B be the adjacency matrices of G_A and G_B.
- Let S be the similarity matrix:

$$S = \begin{pmatrix} s(a_1, b_1) & \cdots & s(a_n, b_1) \\ \vdots & & \vdots \\ s(a_1, b_m) & \cdots & s(a_n, b_m) \end{pmatrix}.$$

- S is computed iteratively:

$$S \leftarrow \frac{BSA^T + B^T SA}{\|BSA^T + B^T SA\|}.$$

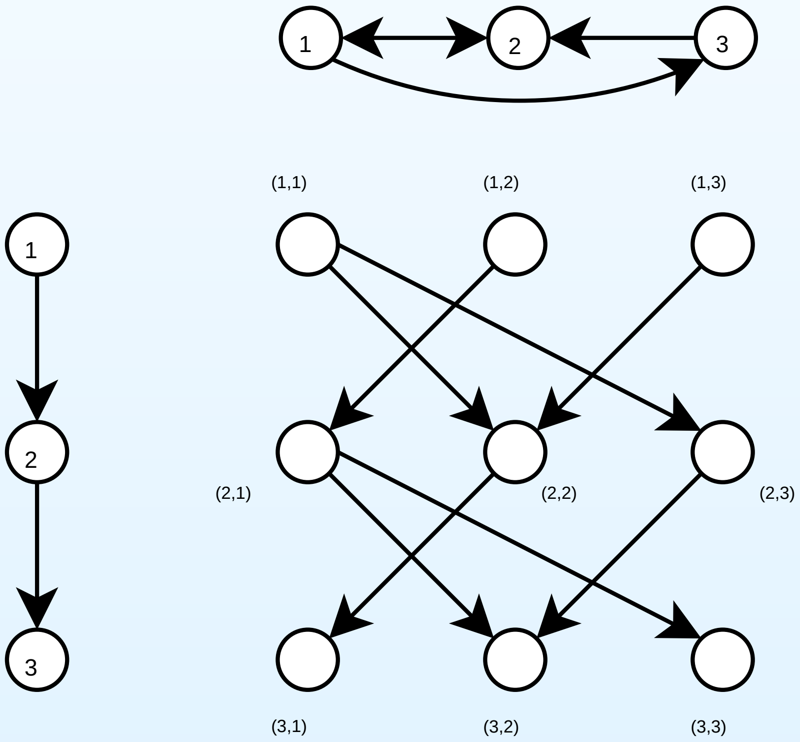
- Convergence concerns: see later.

Computation of the similarity scores

Propagation of scores in the product graph

- Let $G_A \times G_B$ be the product graph and $A \otimes B$ its adjacency matrix.
- The similarity scores are propagated from pair to pair in $G_A \times G_B$.

$$s \leftarrow \frac{(A \otimes B + A^T \otimes B^T)s}{\|(A \otimes B + A^T \otimes B^T)s\|}$$



Computation of the similarity scores

Convergence concerns

The iteration $s_{k+1} = \frac{(A \otimes B + A^T \otimes B^T) s_k}{\|(A \otimes B + A^T \otimes B^T) s_k\|}$ does not always converge!

- **One solution** [Blondel et al. 2002]
  - $A \otimes B + A^T \otimes B^T$ is symmetric
    $\Rightarrow$ each of the subsequences $\{s_{2k}\}_k$ and $\{s_{2k+1}\}_k$ converges.
  - Let $s_{\text{even}}(s_0)$ and $s_{\text{odd}}(s_0)$ these limits.
  - The limit $s_{\text{even}}(\mathbf{1})$ has a nice maximizing property.
  - $s_{\text{even}}(\mathbf{1}) = \lim_{k \to \infty} \dfrac{(A \otimes B + A^T \otimes B^T)^{2k} \mathbf{1}}{\|(A \otimes B + A^T \otimes B^T)^{2k} \mathbf{1}\|}$
    is chosen as the similarity scores vector.

Computation of the similarity scores

Convergence concerns

- **Another solution** [Melnik et al. 2004]
  - Change the iteration formula for

$$s_{k+1} = \frac{(A \otimes B + A^T \otimes B^T)s_k + d}{\|(A \otimes B + A^T \otimes B^T)s_k + d\|}.$$

  - Convergence OK for $d > 0$. [Krause U. 1986]
  - If $d = \varepsilon \mathbf{1}$ then $s_* \approx \dfrac{s_{\text{even}}(\mathbf{1}) + s_{\text{odd}}(\mathbf{1})}{2}$.

Computation of the similarity scores

Convergence concerns

- **Another solution** [Melnik et al. 2002]
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$$s_{k+1} = \frac{(A \otimes B + A^T \otimes B^T)s_k + d}{\|(A \otimes B + A^T \otimes B^T)s_k + d\|}.$$

  - The similarity vector s_* is the solution of

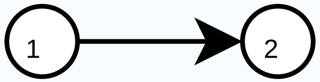
$$\rho(A + dc_*^T)s_* = (A + dc_*^T)s_*$$

with $c_* = \arg\max \rho(A + dc^T)$ on $\{c \geq 0 : \|c\|^D = 1\}$.

[Blondel, N., Van Dooren]

Applications

Hub and authority scores for web searching

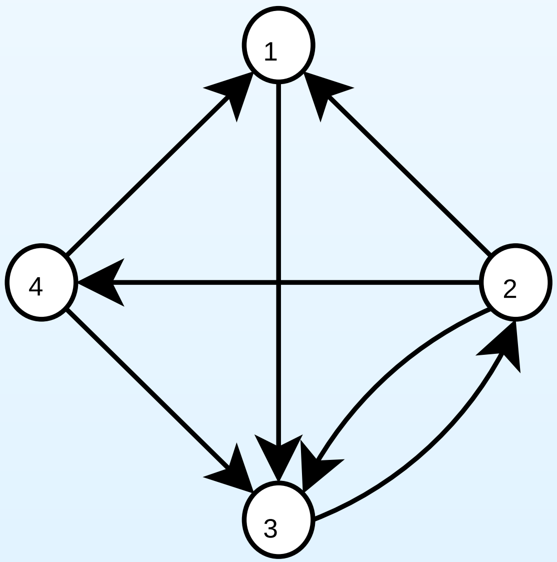
- If G_A is the graph 

the similarity scores give the hub and authority scores.

[Kleinberg 1999]

[Blondel et al. 2004]

- Hub score of a node of G_B = similarity score with node 1 of G_A
- Authority sc. of a node of G_B = similarity sc. with node 2 of G_A

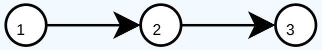


$$S = \begin{pmatrix} (hub) & (auth) \\ 0.2319 & 0.4179 \\ 0.5211 & 0.0000 \\ 0.0000 & 0.5211 \\ 0.4179 & 0.2319 \end{pmatrix}$$

Applications

Synonym extraction and matching of two relational schemas

Some applications of the similarity score:

- Automatic extraction of synonyms:
  - G_A is the graph 
  - G_B a graph constructed from a dictionary.

[Senellart, Blondel 2003]
[Blondel et al. 2004]

- Matching elements of two data schemas:
  - transform the databases in graphs,
  - compute the similarity scores,
  - try to find a good matching.

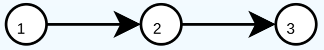
[Melnik et al. 2002]

Examples

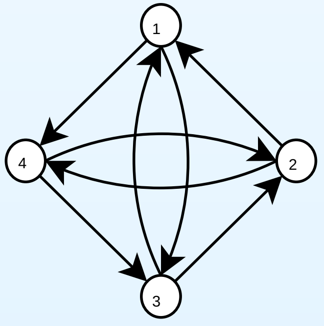
Self similarity

Compare nodes of a graph with nodes of the same graph:

- Path graph: S is diagonal



- Cycle or regular graph: all entries of S are equal



Some limitations

This definition of similarity is still not totally satisfactory

- *Self similarity:*
  the similarity matrix is not always diagonally dominant.

- Similarity matrix does not allow *global comparison* of two graphs.

References

- V. D. Blondel, A. Gajardo, M. Heymans , P. Senellart, and P. Van Dooren, *A measure of similarity between graph vertices: Applications to synonym extraction and web searching*, SIAM Rev. **46** (2004), no. 4, 647–666.
- V. D. Blondel, L. Ninove, and P. Van Dooren, *An affine eigenvalue problem on the nonnegative orthant*, to appear in Linear Algebra and its Applications.
- U. Krause, *A nonlinear extension of the Birkhoff-Jentzsch theorem*, J. Math. Anal. Appl. **114** (1986), no. 2, 552–568.
- S. Melnik, H. Garcia-Molina, and E. Rahm, *Similarity flooding: A versatile graph matching algorithm and its application to schema matching*, Proc. 18th ICDE Conf., 2002.
- P. Senellart and V. D. Blondel, *Automatic discovery of similar words*, ch. 2 in Survey of Text Mining. Clustering, classification, and retrieval, Michael Berry (Ed), pp. 25–44, Springer-Verlag, 2003.

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Large Graphs and Networks
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