Tensor SimRank for Heterogeneous Information Networks

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ABSTRACT
We propose a generalization of SimRank similarity measure for heterogeneous information networks. Given the information network, the intraclass similarity score \( s(a, b) \) is high if the set of objects that are related with \( a \) and the set of objects that are related with \( b \) are pair-wise similar according to all imposed relations.

Categories and Subject Descriptors
[Information systems]: Retrieval models and ranking—Similarity measures

General Terms
SimRank, Probabilistic SVD, Tensor, Low-rank approximation

1. INTRODUCTION
Most data in the modern world can be treated as an information network, thus network node similarity measuring has wide range of applications: search [1], recommendation systems [2], research publication networks analysis [3], biology [4], transportation and logistics [5] and others.

Consider a semantic network: set of types \( T \), each type \( t \in T \) is a set of entities; set of relations \( R \), each relation is 2-order predicate defined on two types from \( T \):

\[ R \ni r_{tp} : t \times p \rightarrow \{1, 0\}, t, p \in T, \]

both types in relation can be equal \((r_{tp} : t \times t \rightarrow \{0, 1\})\), few relations can share the same pair of types \((\exists r_{1p}^{(1)} \neq r_{2p}^{(2)} \in [0, 1]^{t \times p})\). That structure may be considered as a graph with colored vertices and colored edges: vertex color is its entity type, edge color corresponds to a relation.

The question that we address is how to define similarity functions

\[ s_t : t \times t \rightarrow \mathbb{R}, \quad \forall t \in T, \]

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21st ACM SIGKDD ’15 Sydney
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A Type of: devised structured activity
Instance of: candidate KB completeness node, clarifying collection type, type of object, type of temporally stuff-like thing
Subtypes: board game, brand name game, card game, child’s game, coin-operated game, dice game, electronic game, fantasy sports, game for two or more people, game of chance, guessing game, memory game, non-competitive game, non-team game, outdoor game, party game, puzzle game, role-playing game, sports game, table game, trivia game, word game
Instances: ducks and drakes, ultimate frisbee, darts, pachinko, Crossword Puzzle Activity CW, pool, Snooker, mini golf

Figure 1: OpenCyc ontology node of concept "Game"

that would reflect the closeness of objects based on "similarity of relations" they enter, and at the same time not mixing different relations as soon as "objects of different types and links carry different semantic meanings, and it does not make sense to mix them to measure the similarity without distinguishing their semantics" [6].

1.1 Related work
The basic graph structure similarity measure is the classical SimRank [4] over a homogeneous graph \( G = (V, E) \) which is defined as follows:

\[ N_G(a) = \{v \in V : (v, a) \in E(G)\}, \]

\[ s(a, b) = \frac{C}{I(a)I(b)} \sum_{w \in N(a)} s(w, v). \]

The main drawback of this approach is that we cannot induce multiple relations or object types, so the only option is mixing them up into blobs "relation exists" and "all objects" that is completely not applicable in the case we have multiple relations with different semantics, for example the OpenCyc ontology node of the concept "Game" (see Figure 1) cannot be easily expressed via a single type of relations and objects.

Personalized PageRank [8] is also often used to measure
similarity in homogeneous graphs:
\[
\pi_a(b) = \varepsilon \delta_a(b) + (1 - \varepsilon) \sum_{(w,b) \in \mathcal{R}} \frac{\pi_a(w)}{\alpha_{w,v}}.
\]
that it same as PageRank, except random jumps are made into some pre-chosen node \(b\), rather than into random node.

Another option is PathRank [6] that measures path-similarity between objects \(a, b\) picked from the same class \(A\) of the heterogeneous information network \(\mathcal{N}\) given a symmetric meta-path \(\mathcal{P}\) (set of paths that satisfy composition of relations \(M_1, M_2, \ldots, M_n\) that \(A \rightarrow M_1 \rightarrow C_1 \rightarrow M_2 \rightarrow C_2 \rightarrow \cdots \rightarrow M_n \rightarrow A\), so \(A\) is the relation between classes \(\mathcal{P}\) that is same as PageRank, except random jumps are made into some pre-chosen node \(b\), rather than into random node.

\[\pi_a(b) = \sum_{\mathcal{P}} \pi_a(w) \text{ for } (w,b) \in \mathcal{R} \text{ and } \alpha_{w,v} \]

That approach can handle several relations and object types and is very useful when we know the structure of relations we want our similarity measure to be based on. In case we want just to "put our relations into a black box" that would find similarity that would capture all network relations as a whole, we might want to use something different. Recently, an approach [6] for building an optimal linear combination of meta-paths has been proposed.

There are several works on measuring similarity between objects from different classes, see, for example [10].

2. TENSOR SIMRANK

2.1 Problem statement

Let us consider a function \(s_t(a,b)\) that assigns similarity score for two objects from the same class \(t\) as follows: objects \(a, b \in t \in \mathcal{T}\) are similar (value \(s_t(a,b)\) is high) if they relate to objects which are similar too. That interdependence can be expressed via the following definition:

\[N_{tp}(a) = \{b \in p | r_{tp}(a, b) = 1\},\]
\[s_t(a, b) = \frac{1}{Z} \sum_{r_{tp} \in R} w(r_{tp}) \sum_{c \in N_p(a)} \sum_{d \in N_p(b)} s_p(c, d),\]
where \(r_{tp}\) is the relation between classes \(t, p \in \mathcal{T}\). \(N_{tp}\) is the neighbourhood function that returns set of objects from the class \(p\) that are related to the object \(a\) via the relation \(r_{tp}\). \(w(r_{tp})\) are the weights corresponding to the relation \(r_{tp}\). \(Z\) is the normalization constant.

This can be rewritten as a Tensor SimRank equation:

\[s_{\alpha \beta} = \sum_{\gamma} w_{\alpha \beta \gamma} r_{\alpha \beta \gamma} s_{\alpha \beta},\]
\[s = \text{diag}(\{s_t\}_{t \in \mathcal{T}}), \quad s_{\alpha \alpha} = 1,\]
where \(s\) is a block-diagonal matrix (one block per each entity type), \(w\) are the relation weights, \(r_{\alpha \beta \gamma}\) are the stochastic relation tensors\(^1\) (which have non-zero blocks where relations exist).

\(^1\)We have to use tensors instead of matrices to have multiple relations on the same pair of classes

Similarity scores between elements of different classes are equal to zero by the definition. Relation between objects of unrelated classes is equal to zero by definition too. Equation (1) is basically the classical SimRank equation with the adjacency tensor instead of the adjacency matrix: each non-zero layer of tensor encodes some relation on the same pair of types. If one has more than a single relation between types \(p, t \in \mathcal{T}\), then \(r\) would have multiple non-zero layers on the intersection of indices associated with the classes \(t, p\) — one adjacency matrix per layer. In (1) the index \(\gamma\) stands for (weighted) summation over all layers of the tensor. That can be equivalently rewritten explicitly:

\[S = \sum_{\gamma} w_{\gamma} W_{\gamma} S W_{\gamma}^T + D,\]
where the diagonal matrix \(D\) has to be chosen in such a way that \(\text{diag}(S) = I\).

2.2 Computational algorithm

Simple iterations for (1) are computationally demanding due to large-scale matrix-by-matrix products, thus we propose a method that exploits the fact that \(s\) is block diagonal and \(r\) is a three-dimensional block tensor with size of the last dimension (number of layers) much less then the overall amount of objects. On each iteration \(k\) for each \(r \in \mathcal{R}\) we recompute \(s_t\) updates independently (assuming all other \(s_j\) fixed), see Algorithm 1.

\begin{algorithm}
\caption{Idea under Tensor SimRank}
\begin{algorithmic}
\State Data: \(\mathcal{T}\) - classes, \(\mathcal{R}\) - relations
\State Result: \(S = \{s_t(a,b)\}_{t \in \mathcal{T}}\)
\Repeat
\For {\(s_t \in S\)}
\State assume all \(S \setminus s_t\) fixed
\EndFor
\For {\(r \in \mathcal{R}: r_{tp}: t \times p \mapsto \{0, 1\}\)}
\For {\((a, b) \in t\) }
\For {\((c, d) \in p\) }
\State \(s_{t_{\text{next}}}(a, b) = s_{t_{\text{next}}}(a, c)s_{p}(c, b)r_{p}(b, d)\)
\EndFor
\EndFor
\EndFor
\Until {\(\sum_{t} \|s_t - s_{t_{\text{next}}}\| < \delta\)}
\end{algorithmic}
\end{algorithm}

So we just update the similarity score for each class assuming all other classes similarities are fixed in a way that the objects from the target class \((t)\) that are related to objects from some other class \((c, d) \in p\) that are close \((s_p(c, d)\) is high) become closer too \((s_t(a, b)\)).

To show actual vectorized algorithm of similarity computation, let us introduce some additional notations: set of entity types \(\mathcal{T} = \{t_i\}_{i=0}^N\) each entity type \(t\) is a set of entities, set of symmetric relation functions \(\mathcal{R} = \{r_{tp}(j)\}_{j=0}^N\) where \(r_{tp}(j): t \times p \mapsto \{0, 1\}\), \(t, p \in \mathcal{T}\), \(j\) is the order; column-stochastic matrix of pairwise impacts (weights) \(w \in \mathbb{R}^{N \times N}\) operator \(W: r_{tp}^{(j)} \rightarrow \mathbb{R}^{[j] \times |p|}\) that maps relation
into corresponding column-stochastic adjacency matrix. If $r_{tp}$ is not defined for some $(t, p) \in \mathcal{T}^2$, then $w_{tp} = 0$.

**Algorithm 2: Vectorised Tensor SimRank for HSM**

Data: $\mathcal{T}$ - classes, $\mathcal{R}$ - relations, $w$ - relation weights

Result: $S = \{s_t(a, b)\}_{t \in \mathcal{T}}$

for $t \in \mathcal{T}$ do
  $s_t^{(0)} = I$
  $k = 0$
  repeat
    for $t \in \mathcal{T}$ do
      $s_t^{(k+1)} = s_t^{(k)} - \text{diag}(s_t^{(k)}) + I$
    end
    $k = k + 1$
  until $\sum_{t \in \mathcal{T}} \|s_t^{(k+1)} - s_t^{(k)}\| \leq \varepsilon$;

To achieve better results (see above) on sparse relations we adopted the Low-Rank SimRank approximation [11] that uses Probabilistic Singular Value Decomposition [12] to perform fast approximate projections on low-rank matrix manifold at each step of the iterative process (Algorithm 3).

The only difference with Algorithm 2 is that on each step we perform probabilistic SVD decomposition of the matrix $S - I$, so that $S \approx I + UDI^T$, and project it onto the manifold of matrices of rank $a_t$.

**Algorithm 3: Low-rank Tensor SimRank for HSM**

Data: $\mathcal{T}$ - classes, $\mathcal{R}$ - relations, $w$ - relation weights, $\{a_t\}$ - approximation ranks

Result: $S = \{s_t(a, b)\}_{t \in \mathcal{T}}$

for $t \in \mathcal{T}$ do
  $s_t^{(0)} = I$
  end

$k = 0$
$u_t = 0$
$d_t = 0$
repeat
  for $t \in \mathcal{T}$ do
    $s_t^{\text{new}} = s_t^{\text{old}} - T$
    $u_t, d_t = \text{ProbabilisticSVD}(s_t^{\text{new}}, a_t)$
  end
  $s_t^{(k+1)} = s_t^{\text{new}} + I$
  $k = k + 1$
until $\sum_{t \in \mathcal{T}} \|s_t^{(k+1)} - s_t^{(k)}\| \leq \varepsilon$;

which can be generalized to the tensor case as

$$S = c \sum_{\gamma} w_{\gamma} W_{\gamma} W_{\gamma}^T + (1 - c)I,$$

and a fixed-point iteration converges [13] if:

$$\sum_{\gamma=1}^{N} w_{\gamma} \|W_{\gamma}\|^2 \leq \frac{\|W_{\gamma}\|_{\text{stochastic}}}{\varepsilon} \sum_{\gamma} w_{\gamma} \leq 1.$$

We conjecture that fixed-point iterations for (3) converge if:

1. Each $W_{\gamma}$ is stochastic
2. $\sum_{\gamma} w_{\gamma} = 1$

In the simplest form (we have no preferences among relations and classes) it reduces to (relations weight):

$$w_{tp} = \frac{1}{\sum_{m} \|r_{tm}^{(i)}\|_{\mathcal{R}}}.$$

**3. COMPUTATIONAL EXPERIMENT**

**3.1 Synthetic data: convergence test**

To test convergence conditions we conducted series of tests on randomly generated sparse networks with different number of classes: $K \in \{3, 5, 7, 10\}$ and with randomly chosen number of objects in each $N_{\text{real}} \in U_{(N/2, N)}$, $N \in \{10, \ldots, 100\}$, full network of relation types (all possible types relations exist) with $2 \min(N_{\text{real}}, N_{\text{real}}^T)$ randomly chosen edges in each and default $w$ matrix (no priority). All generated networks successfully converged that illustrates that convergent sufficient conditions listed in previous section were adequate, see Figures 2, 3.

$$\text{vec}(ABC) = (C^T \otimes A)\text{vec}(B)$$
3.2 Synthetic data: similarity reconstruction

To determine if model is capable of similarity reconstruction we generated a tree graph from randomly distributed points on a plane and tested if model can reconstruct points spatial similarity basing only on their relations.

On Figure 4 blue point represent 0-level point that are connected to 1-level point (red), that are connected to 2-level points (green).

We have measured the following similarity reconstruction \( \tilde{S} \) quality compared to real \( S \) obtained from generated point coordinates:

\[
Q(S, \tilde{S}) = \sum_a \sum_b \sum_c [S_{ab} < S_{ac} \text{ and } \tilde{S}_{ab} < \tilde{S}_{ac}] / \sum_i \sum_j \sum_k 1
\]

that actually shows how many "a is closer to c then to b" relations were preserved.

From Figure 3 one can see that at level \( r \approx 0.3 \) model gets saturated, but at the level \( r \approx 0.15 \) models that use low-rank version of Tensor SimRank perform way better than the "pure" algorithm. The numbers in the brackets denote the dimensionality of the matrix space into which the similarity matrices were projected on each step (rank of approximation).

3.3 Book-Crossing Dataset test

The model was run on subsample from the Book-Crossing Dataset [14]. We have extracted only those authors who had highest (top100) number of books in the collection. The final network had the following structure:

\[
T = \{ \text{Book, Author, Year, Publisher} \}
\]

\[
R = \{ \text{isAuthorOf}(\cdot, \cdot), \text{publishedBy}(\cdot, \cdot), \text{publishedIn}(\cdot, \cdot) \}
\]

\#Book = 3625, \#Author = 99, \#Year = 65, \#Publisher = 554

Model convergence is shown on Figure 3.3, where successful convergence to the best possible low-rank approximation can be seen. The similarity structure is clearly visible on Year similarity matrix heatmap (Figure 3.3). We expect diagonal dominance as soon as temporarily close years should be more or less similar in terms of authors and publishers characteristic of that period. Tables 1 and 2 are examples of "closest book" requests, we want to notice that no NLP-preprocessing was conducted, nevertheless model treated books from same storybook as similar basing on author/publisher/year similarities.

4. DISCUSSION AND FURTHER WORK
Proposed model can be used in various problem areas where most of the information is available in the form of relations between entities rather than features of individual entities and no trivial vector representation of those entities can be induced. One can use the vector representation

$$[s_{ij}] = [\delta_{ij} + [u_{ik}] [d_{ij}] [u_{lj}],$$

to embed the notion of relations into classical machine learning algorithms. Also, the proposed model can be used for relation generalisation, that might give interesting results since we work on heterogeneous graphs.

Further model improvements might also include treating relations as objects too (probably, via heterogeneous hyper-graphs) and defining similarity matrix on relations.

5. CONCLUSION

This paper proposes the generalization of SimRank for heterogeneous networks and a method for its computation that exploits the fact that the resulting similarity matrix is block-diagonal, thus its components might be computed in an iterative fashion. The convergence conditions are proposed and successfully tested. Few perspective application areas are suggested.

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