Loss Function for Skip-Gram methods (II)

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Recall from last time

Algorithm 1 DeepWalk(G, w, d, γ, t)

Input: graph $G(V, E)$
window size w
embedding size d
walks per vertex γ
walk length t

Output: matrix of vertex representations $\Phi \in \mathbb{R}^{|V| \times d}$

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Initialization: Sample Φ from U^{|V|×d}
Build a binary Tree T from V
for i = 0 to γ do
    O = Shuffle(V)
    for each v_i ∈ O do
        W_{v_i} = RandomWalk(G, v_i, t)
        SkipGram(Φ, W_{v_i}, w)
    end for
end for
```

DeepWalk Skip-gram update procedure

Algorithm 2 SkipGram(Φ, $\mathcal{W}_{v_i}$, w)

for each $v_j \in \mathcal{W}_{v_i}$ **do**
  for each $u_k \in \mathcal{W}_{v_i}[j-w : j+w]$ **do**
    $J(\Phi) = -\log \Pr(u_k \mid \Phi(v_j))$
    $\Phi = \Phi - \alpha * \frac{\partial J}{\partial \Phi}$
  end for
end for

- given current representation of vertex $v_j, \Phi(v_j) \in \mathbb{R}^d$, want to maximize the probability of seeing its neighbors in the walk

Objective

- Basic definition:

$$\Pr(u_k|\Phi(v_i)) = \frac{\exp(\Phi(u_k)^T\Phi(v_i))}{\sum_{1\leq v_j\leq |V|}\exp(\Phi(v_j)^T\Phi(v_i))}$$

and yes this probably can be written in the matrix form, leading to the question of whether we really have to do one node at a time

Computational challenge

- it really depends on size of $|V|$
- if $|V|$ is in the range of $\geq 10^5$. computing this at each round could be very expensive
- however, if your graph doesn't have as many nodes (say < 5000) perhaps simply computing like this is enough

There are ways to efficiently approximate the softmax:

- hierarchical softmax
- negative sampling / Noise contrastive estimation

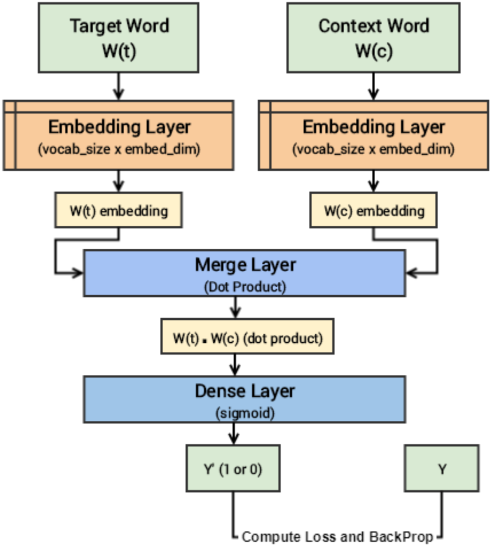
Issue from last time

Would maximizing

$$\Pr(u_k|\Phi(v_i)) = \frac{\exp(\Phi(u_k)^T\Phi(v_i))}{\sum_{1\leq v_j\leq|V|}\exp(\Phi(v_j)^T\Phi(v_i))}$$

cause the learnt vectors to blow up?

The neural network



Noise Contrastive Estimation (NCE) / Negative sampling

- so far, only maximizing probability of word/node within context
- here, aims at maximizing the similarity of the words in the same context and minimizing it when they occur in different contexts
- idea: get a noise distribution by negative sampling from unrelated parts of the graph

Some notation in graphs

- k-step transition matrix: A^k
  Quick quiz: if A is the adjacency matrix, what does A^k tell us?
- Pr(go from node v_i to node v_j in k steps) $= A^k_{i,j}$,
  let this be denoted by $p_k(v_j|v_i)$
- let $p_k(V)$ be some distribution over vertices in the graph
  (I actually couldn't find more details on this)
- sample a vertex c according to $p_k(V)$ – negative sampling, then
  $p_k(c) = \frac{1}{N} \sum_{v_i} A^k_{v_i,c}$

Loss function

- define local loss over a specific pair (v_i, v_j):

$$\begin{aligned} L_k(v_i, v_j) &= p_k(v_j|v_i) \cdot \log(\sigma(\Phi(v_i) \cdot \Phi(v_j)) + \lambda \cdot p_k(v_j) \cdot \log \sigma(-\Phi(v_i) \cdot \Phi(v_j)) \\ &= A^k_{v_i, v_j} \cdot \log(\sigma(\Phi(v_i) \cdot \Phi(v_j)) + \lambda \cdot p_k(v_j) \cdot \log \sigma(-\Phi(v_i) \cdot \Phi(v_j)) \end{aligned}$$

  where the second term refers to the probability of v_j being negatively sampled, λ: hyperparameter indicating no. of negative samples
- k-step loss function of a node:
  $L_k(v_i) = \sum_{v_j \neq v_i} L_k(v_i, v_j)$
- k-step loss function over whole graph
  $L_k = \sum_{v \in V} L_k(v)$

Back propagation

- let $z = \Phi(v_i) \cdot \Phi(v_j)$, and set $\frac{\delta L_k}{\delta z} = 0$
  we get
  $$\Phi(v_i) \cdot \Phi(v_j) = \log\left(\frac{A^k_{v_i,v_j}}{\sum_w A^k_{w,v_j}}\right) - \log\frac{\lambda}{N}$$
  Let this matrix be Y^k
  (I didn't do the math...perhaps you can try)
- For SVD, we want at least a semi positive-definite matrix, so we remove the negative values in Y^k by letting $X^k = max(Y^k, 0)$,
  so $X^k_{i,j} \approx \Phi(v_i) \cdot \Phi(v_j)$ after replacing the negative entries with 0
- X^k can then be factored with SVD or other methods to get $X^k \approx U\Sigma V$
- thus $\Phi \approx U(\Sigma)^{\frac{1}{2}}$

GraRep - Algorithm

GraRep Algorithm

Input

Adjacency matrix S on graph
Maximum transition step K
Log shifted factor β
Dimension of representation vector d

1. Get k-step transition probability matrix A^k

Compute $A = D^{-1}S$
Calculate $A^1, A^2, \ldots, A^K$, respectively

2. Get each k-step representations

For $k = 1$ to K

2.1 Get positive log probability matrix
calculate $\Gamma_1^k, \Gamma_2^k, \ldots, \Gamma_N^k$ ($\Gamma_j^k = \sum_p A_{p,j}^k$) respectively
calculate $\{X_{i,j}^k\}$

$$X_{i,j}^k = \log\left(\frac{A_{i,j}^k}{\Gamma_j^k}\right) - \log(\beta)$$

assign negative entries of X^k to 0

2.2 Construct the representation vector W^k
$[U^k, \Sigma^k, (V^k)^T] = SVD(X^k)$
$W^k = U_d^k (\Sigma_d^k)^{\frac{1}{2}}$

End for

3. Concatenate all the k-step representations

$W = [W^1, W^2, \ldots, W^K]$

Output

Matrix of the graph representation W

Other ideas

- for vertex-vertex relationship, it doesn't have to be dot-product
- other methods include but not limited to
  - common neighbors $|N(u) \cap N(v)|$
  - Jaccard's coefficient $\dfrac{|N(u) \cap N(v)|}{|N(u) \cup N(v)|}$
  - Adamic-Adar score $\sum_{t \in |N(u) \cap N(v)|} \dfrac{1}{\log |N(t)|}$
  - Preferential attachment $|N(u)| \cdot |N(v)|$

  for vertex pair u, v with neighbor set $N(u)$ and $N(v)$

Summary

- random walk is a way to capture local (and by induction, global) structure of a graph
- this class of methods is non-Euclidean, and loss function is different
- suitable for scenarios where the underlying graphical structure is known, and we want to be able to learn node representation or infer nodes in close neighborhood with ease in a particularly large graph

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Thank you for listening!

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