Revisiting Semi-Supervised Learning with Graph Embeddings

基于图嵌入的半监督学习

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Main Work

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The main highlight of our work is to incorporate embedding techniques into the graph-based semi-supervised learning setting.

What Is Semi-Supervised Learning?

Let L and U be the number of labeled and unlabeled instances. Let $\mathbf{x}_{1:L}$ and $\mathbf{x}_{L+1:L+U}$ denote the feature vectors of labeled and unlabeled instances respectively. The labels $y_{1:L}$ are also given.

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There are two learning paradigms, transductive learning and inductive learning.

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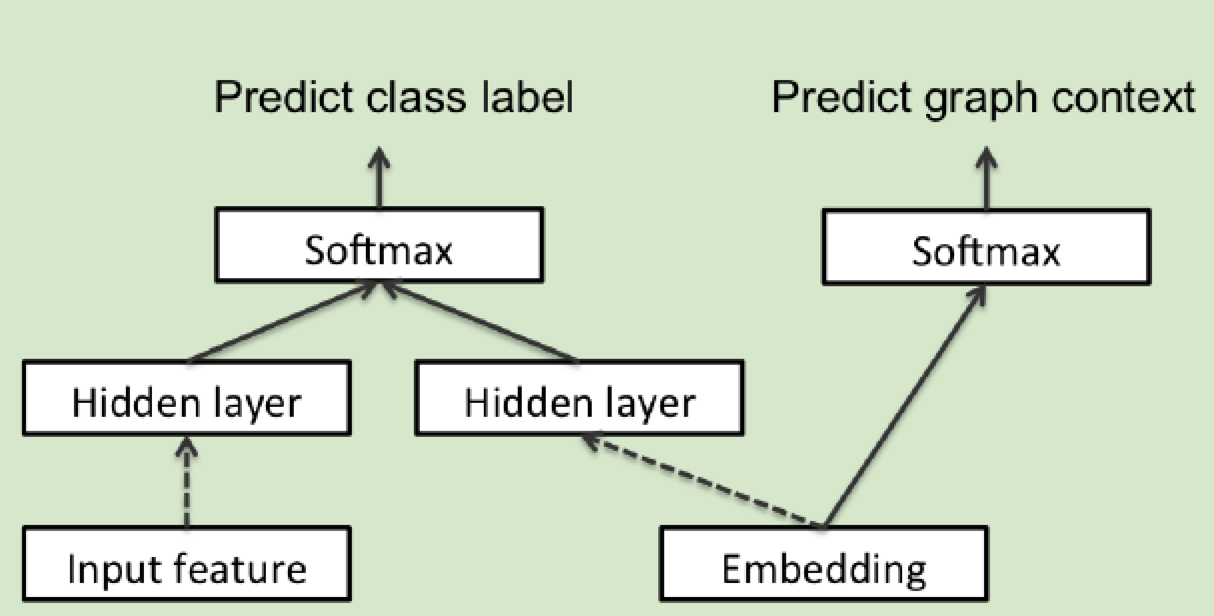
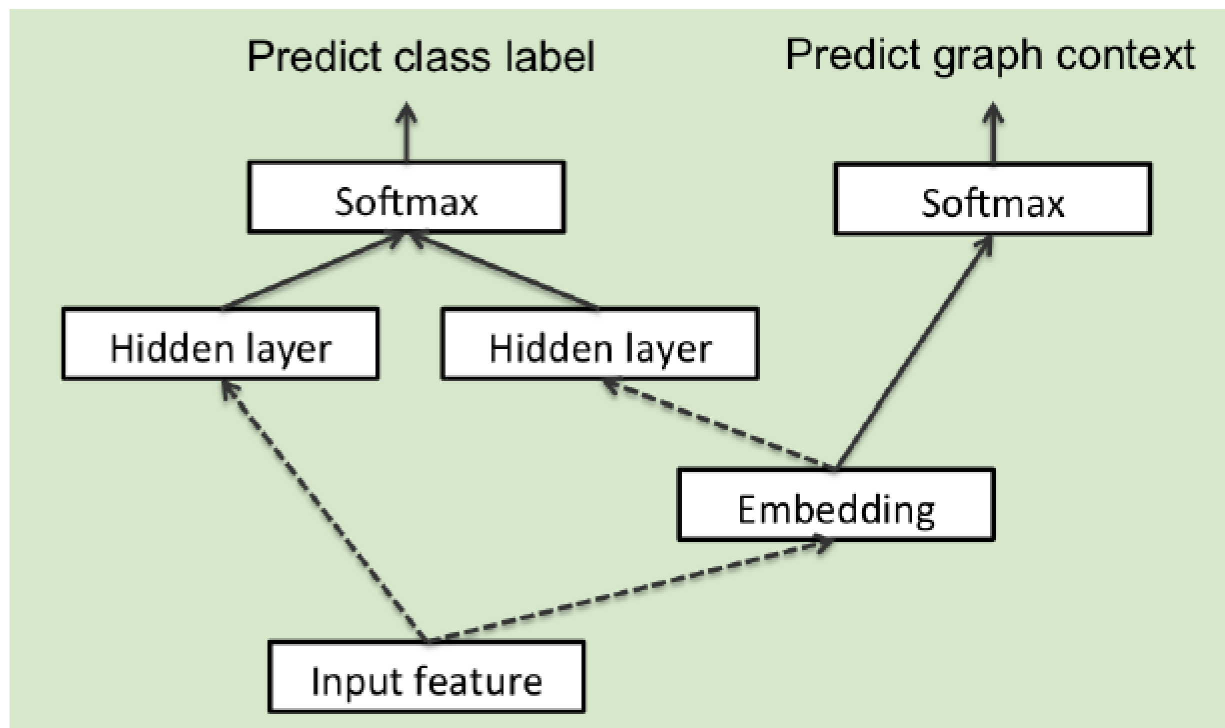
Inductive learning

on the other hand, aims to learn a parameterized classifier f that is generalizable to unobserved instances.



(a) Transductive Formulation



(b) Inductive Formulation

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In addition to labeled and unlabeled instances, a graph, denoted as a $(L+U) \times (L+U)$ matrix A, is also given to graph-based semi-supervised learning methods.

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In this paper,
we mainly focus on the setting that a graph is explicitly given and represents additional information not present in the feature vectors

(e.g., the graph edges correspond to hy- perlinks between documents).

The Loss Function

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Generally, the loss function of graph-based semi-supervised learning in the binary case can be written as

$$
\begin{aligned}
& \sum_{i=1}^{L} l(y_i, f(x_i)) + \lambda \sum_{i,j} a_{ij} \| f(x_i) - f(x_j) \|^2 \\
= \; & \sum_{i=1}^{L} l(y_i, f(x_i)) + \lambda \mathbf{f}^T \Delta \mathbf{f} \qquad (1)
\end{aligned}
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The graph Laplacian matrix Δ

$\Delta = A - D$, where D is a diagonal matrix with each entry defined as $d_{ii} = \sum_j a_{ij}$.

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\end{aligned}
$$

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How?

$$\sum_{i,j} a_{i,j} \|f(x_i)-f(x_j)\|^2 =$$

$$\sum_{i,j} a_{i,j} \left(\; f(x_i)^2 + f(x_j)^2 - 2 f(x_i) f(x_j) \; \right) =$$

$$\sum_{i,j} a_{i,j} f(x_i)^2 + \sum_{i,j} a_{i,j} f(x_j)^2 + \sum_{i,j} -2 f(x_i) f(x_j) a_{i,j} =$$

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$$2 [\sum_{i,j} a_{i,j} f(x_i)^2 + \sum_{i,j} - f(x_i) f(x_j) a_{i,j}] =$$

$$(ignore\, 2)$$

$$\sum_{i} f(x_i)^2 \sum_{j} a_{i,j} - \sum_{i} f(x_i) \sum_{j} f(x_j) a_{i,j} =$$

$$\sum_{i} f(x_i)^2 d_{ii} - \sum_{i} f(x_i) \sum_{j} f(x_j) a_{i,j} =$$

$$f^T D f - f^T A f =$$

$$f^T (D-A) f$$

Semi-Supervised Learning with Graph Embeddings

We formulate our framework based on feed-forward neural networks.

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Given the input feature vector $\mathbf{x}$, the k-th hidden layer of the network is denoted as $\mathbf{h}^k$, which is a nonlinear function of the previous hidden layer $\mathbf{h}^{k-1}$ defined as: $\mathbf{h}^k(\mathbf{x}) = \mathrm{ReLU}(\mathbf{W}^k \mathbf{h}^{k-1}(\mathbf{x}) + b^k)$, where $\mathbf{W}^k$ and b^k are parameters of the k-th layer, and $\mathbf{h}^0(\mathbf{x}) = \mathbf{x}$. We adopt rectified linear unit $\mathrm{ReLU}(x) = \max(0, x)$ as the nonlinear function in this work.

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The loss function of our framework can be expressed as

$$\mathcal{L}_s + \lambda \mathcal{L}_u,$$

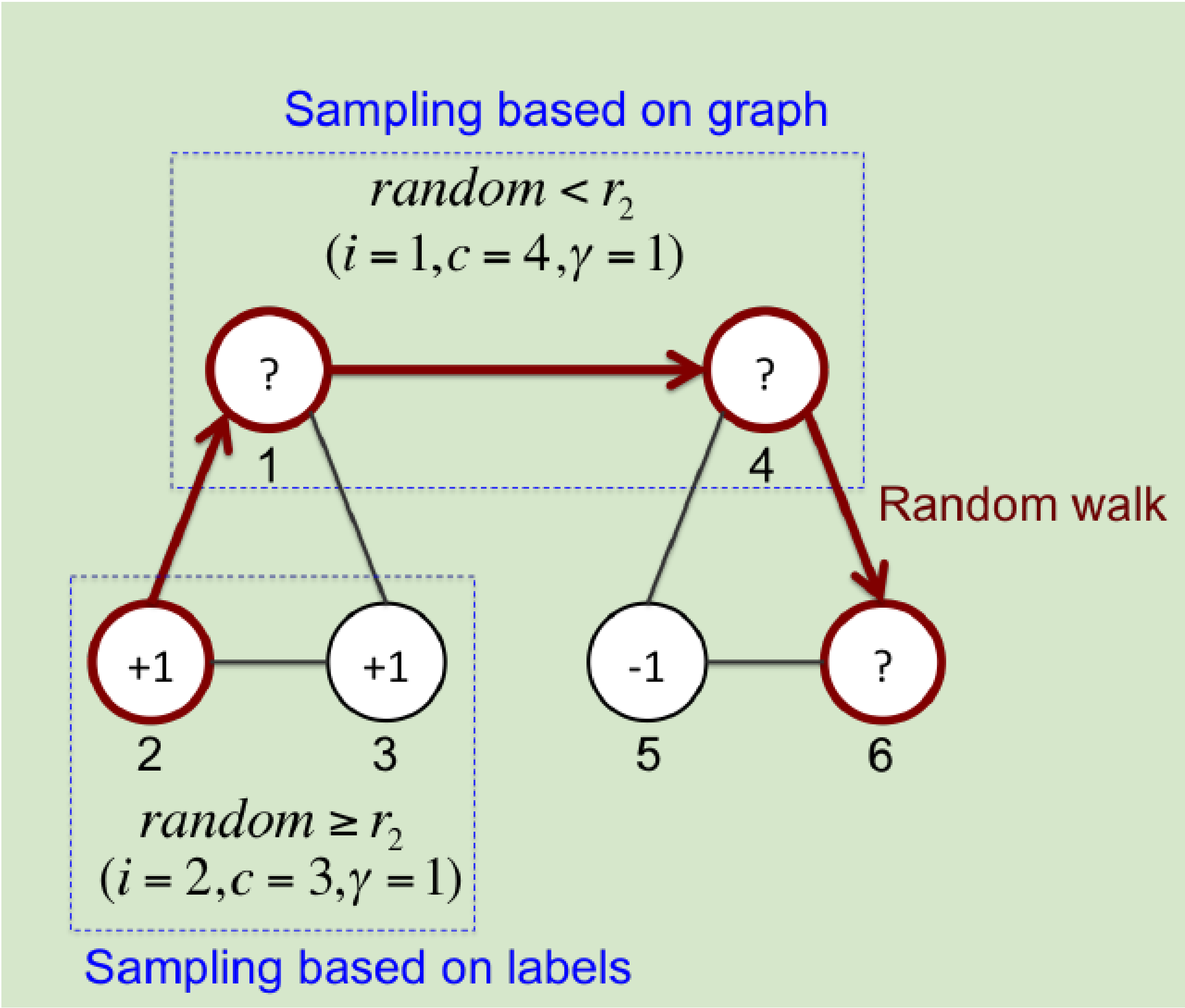
where $\mathcal{L}_s$ is a supervised loss of predicting the labels, and $\mathcal{L}_u$ is an unsupervised loss of predicting the graph context.

Unsupervised Loss

the unsupervised loss with negative sampling can be written as

$$\mathcal{L}_u = -\mathbb{E}_{(i,c,\gamma)} \log \sigma(\gamma \mathbf{w}_c^T \mathbf{e}_i) \quad (3)$$

Unsupervised Loss



Unsupervised Loss

Algorithm 1 Sampling Context Distribution $p(i, c, \gamma)$

Input: graph A, labels $y_{1:L}$, parameters r_1, r_2, q, d
Initialize triplet (i, c, γ)
if $random < r_1$ **then** $\gamma \leftarrow +1$ **else** $\gamma \leftarrow -1$
if $random < r_2$ **then**
  Uniformly sample a random walk S of length q
  Uniformly sample (S_j, S_k) with $|j - k| < d$
  $i \leftarrow S_j, c \leftarrow S_k$
  if $\gamma = -1$ **then** uniformly sample c from $1 : L + U$
else
  if $\gamma = +1$ **then**
    Uniformly sample (i, c) with $y_i = y_c$
  else
    Uniformly sample (i, c) with $y_i \neq y_c$
  end if
end if
return (i, c, γ)

Label Loss

$$p(y|\mathbf{x},\mathbf{e}) = \frac{\exp[\mathbf{h}^k(\mathbf{x})^T, \mathbf{h}^l(\mathbf{e})^T]\mathbf{w}_y}{\sum_{y'} \exp[\mathbf{h}^k(\mathbf{x})^T, \mathbf{h}^l(\mathbf{e})^T]\mathbf{w}_{y'}}, \qquad (4)$$

$[\cdot, \cdot]$ denotes concatenation of two row vectors and $\mathbf{w}$ represents the model parameter.

Label Loss

$$p(y|\mathbf{x}, \mathbf{e}) = \frac{\exp[\mathbf{h}^k(\mathbf{x})^T, \mathbf{h}^l(\mathbf{e})^T]\mathbf{w}_y}{\sum_{y'} \exp[\mathbf{h}^k(\mathbf{x})^T, \mathbf{h}^l(\mathbf{e})^T]\mathbf{w}_{y'}}, \qquad (4)$$

Combined with Eq. (3), the loss function of transductive learning is defined as:

$$-\frac{1}{L}\sum_{i=1}^{L} \log p(y_i|\mathbf{x}_i, \mathbf{e}_i) - \lambda \mathbb{E}_{(i,c,\gamma)} \log \sigma(\gamma \mathbf{w}_c^T \mathbf{e}_i),$$

Inductive Formulation

Replacing $\mathbf{e}_i$ in Eq. (3) with $\mathbf{h}^{l_1}(\mathbf{x}_i)$, the loss function of inductive learning is

$$-\frac{1}{L}\sum_{i=1}^{L}\log p(y_i|\underline{\mathbf{x}_i}) - \lambda\mathbb{E}_{(i,c,\gamma)}\log\sigma(\gamma\mathbf{w}_c^T\underline{\mathbf{h}^{l_1}(\mathbf{x}_i)})$$

Model Training

Algorithm 2 Model Training (Transductive)

Input: A, $\mathbf{x}_{1:L+U}$, $y_{1:L}$, λ, batch iterations T_1, T_2 and sizes N_1, N_2

repeat

  for $t \leftarrow 1$ **to** T_1 **do**

    Sample a batch of labeled instances i of size N_1

    $\mathcal{L}_s = -\frac{1}{N_1}\sum_i p(y_i|\mathbf{x}_i, \mathbf{e}_i)$

    Take a gradient step for $\mathcal{L}_s$

  end for

  for $t \leftarrow 1$ **to** T_2 **do**

    Sample a batch of context from $p(i, c, \gamma)$ of size N_2

    $\mathcal{L}_u = -\frac{1}{N_2}\sum_{(i,c,\gamma)} \log \sigma(\gamma \mathbf{w}_c^T \mathbf{e}_i)$

    Take a gradient step for $\mathcal{L}_u$

  end for

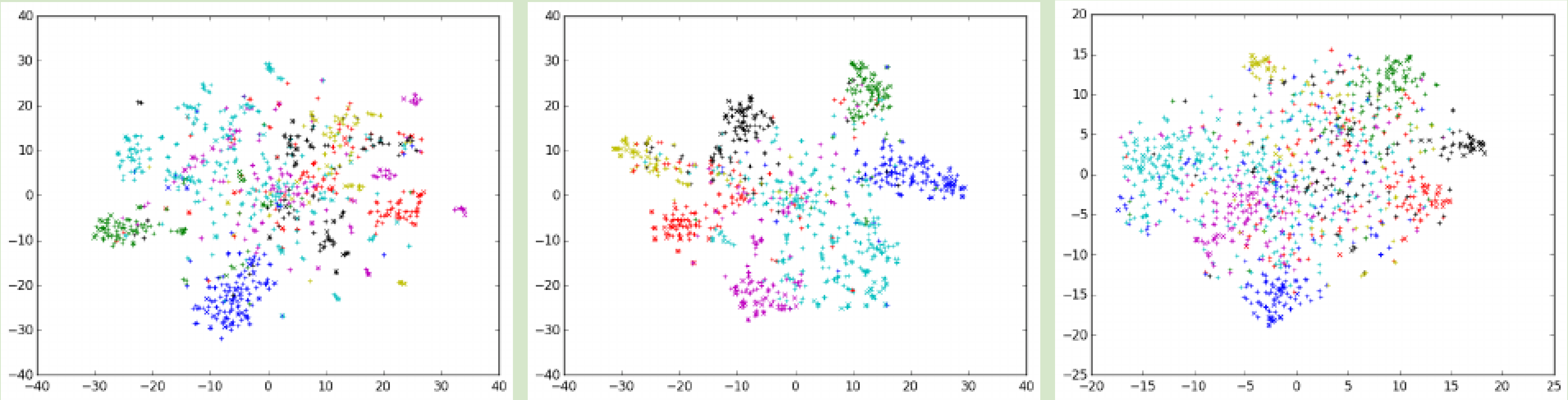
until stopping

Supervised Training on label

SGD with mini-batch mode

Unsupervised Training on context

Experiments



(a) GraphEmb (b) Planetoid-T (c) SemiEmb

Figure 3. t-SNE Visualization of embedding spaces on the Cora dataset. Each color denotes a class.

One More Thing

Thanks for Listening

Preferences

- [1] 《Revisiting Semi-supervised Learning with Graph Embeddings. Zhilin Yang, William W. Cohen, Ruslan Salakhutdinov. ICML 2016.》
- [2]