Deep Learning - Foundations and Concepts

Chapter 13. Graph Neural Networks

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Outline

Machine learning on graphs

There are many kinds of applications that we might wish to address using graph-structured data:

- Node prediction: Classify documents according to their topic based on the hyperlinks and citations between the documents.
- Edge prediction (graph completion): Knowing some of the interactions in a protein network and predict the presence of any additional ones.
- Graph prediction: Predict whether a particular molecule is soluble in water.

Graph properties

- A graph $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ consists of a set of nodes or vertices, denoted by $\mathcal{V}$, along with a set of edges or links, denoted by $\mathcal{E}$.
- We index the nodes by $n = 1, \ldots, N$, and we write the edge from node n to node m as (n, m).
- If two nodes are linked by an edge they are called neighbors, and the set of all neighbors of node n is denoted by $\mathcal{N}(n)$.
- For each node n we can represent the corresponding node variables as a D-dimensional column vector x_n and we can group these into a data matrix X of dimensionality $N \times D$.

Adjacency matrix

A convenient way to specify the edges in a graph is to use an adjacency matrix denoted by A:

- To define the adjacency matrix we first have to choose an ordering for the nodes.
- The adjacency matrix has dimensions $N \times N$ and contains a 1 in every location n, m for which there is an edge going from node n to node m, with all other entries being 0.
- We could consider using adjacency matrix directly as the input to a neural network. To do this we could flatten the matrix, for example by concatenating the columns into one long column vector.
- The node ordering invariance should be treated as an inductive bias when constructing a network architecture.

Permutation equivariance

- A permutation π is a bijection from $\{1, \ldots, N\}$ to itself.
- Let $\{e_1, \ldots, e_N\}$ be the standard basis of $\mathbb{R}^N$, given a permutation π, the corresponding permutation matrix P is defined as:
  $P = \begin{pmatrix} e_{\pi(1)} & \cdots & e_{\pi(N)} \end{pmatrix}^T$
- When we reorder the labelling on the nodes of a graph:
  - The data matrix X is changed to $\tilde{X} = P^T X$.
  - The adjacency matrix A is changed to $\tilde{A} = P^T A P$.
  - Any global property of the graph does not depend on node label reordering: $y(\tilde{X}, \tilde{A}) = y(X, A)$.
  - Node predictions should be equivariant with respect to node label reordering: $y(\tilde{X}, \tilde{A}) = P^T y(X, A)$.

Convolutional filters

Consider a convolutional layer using 3×3 filters. The computation performed by a single filter at a single pixel in layer $l+1$ can be expressed as:

$$z_i^{(l+1)} = f(\sum_j w_j z_j^{(i)} + b)$$

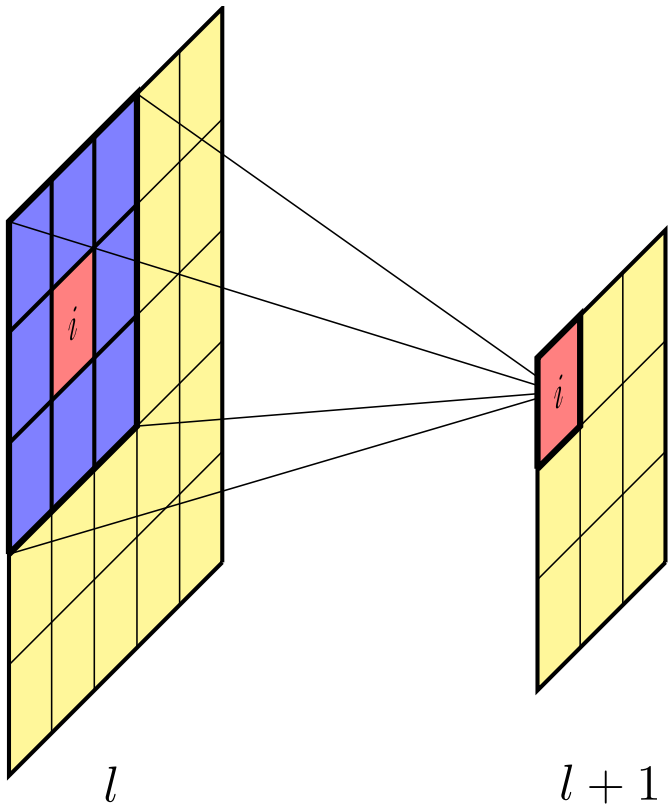
This is not equivariant under reordering of the nodes in layer l. However, we can achieve equivariance with some simple modifications as follows:

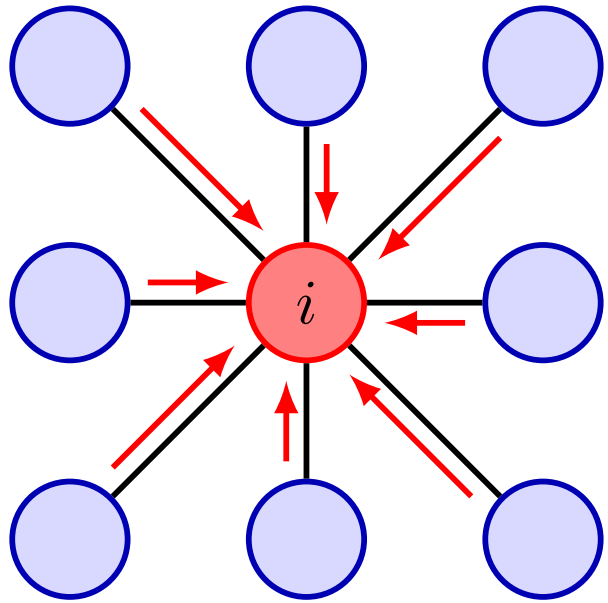
$$z_i^{(l+1)} = f(w_{\text{neigh}} \sum_{j \in \mathcal{N}(i)} z_j^{(l)} + w_{\text{self}} z_i^{(l)} + b)$$

where a single weight parameter w_{neigh} is shared across the neighbors, and node i has its own weight parameter w_{self}.

Convolutional filters

Figure: A convolutional filter for images can be represented as a graph-structured computation





Graph convolutional networks

We can view each layer of processing as having two successive stages:

- Aggregation stage: For each node n, messages are passed to that node from its neighbors and combined to form a new vector $z_n^{(l)}$ in a way that is permutation invariant:
  $z_n^{(l)} = \text{Aggregate}(\{h_m^{(l)} : m \in \mathcal{N}(n)\})$.
- Update stage: The aggregated information from neighboring nodes is combined with local information from the node itself and used to calculate a revised embedding vector for that node:
  $h_n^{(l+1)} = \text{Update}(h_n^{(l)}, z_n^{(l)})$.

Graph convolutional networks

Algorithm 1: Simple message-passing neural network

for $l \leftarrow 0$ **to** $L-1$ **do**

$z_n^{(l)} \leftarrow \text{Aggregate}(\{h_m^{(l)} : m \in \mathcal{N}(n)\})$;

$h_n^{(l+1)} \leftarrow \text{Update}(h_n^{(l)}, z_n^{(l)})$;

end

return $\{h_n^{(L)}\}$;

Aggregation operators

Some simple aggregation functions:

$$\text{Aggregate}(\{h_m^{(l)} : m \in \mathcal{N}(n)\}) = \sum_{m \in \mathcal{N}(n)} h_m^{(l)}$$

$$\text{Aggregate}(\{h_m^{(l)} : m \in \mathcal{N}(n)\}) = \frac{1}{|\mathcal{N}(n)|} \sum_{m \in \mathcal{N}(n)} h_m^{(l)}$$

$$\text{Aggregate}(\{h_m^{(l)} : m \in \mathcal{N}(n)\}) = \sum_{m \in \mathcal{N}(n)} \frac{h_m^{(l)}}{\sqrt{|\mathcal{N}(n)||\mathcal{N}(m)|}}$$

$$\text{Aggregate}(\{h_m^{(l)} : m \in \mathcal{N}(n)\}) = \max(\{h_m^{(l)} : m \in \mathcal{N}(n)\})$$

Aggregation operators

We can introduce learnable parameters by:

- First transforming each of the embedding vectors from neighboring nodes using a multilayer neural network, denoted by MLP_ϕ.
- Then transforming the combined vector with another neural network MLP_θ.

to give an overall aggregation operator:

$$\mathrm{Aggregate}(\{h_m^{(l)} : m \in \mathcal{N}(n)\}) = \mathrm{MLP}_\theta\Big(\sum_{m \in \mathcal{N}(n)} \mathrm{MLP}_\phi(h_m^{(l)})\Big)$$

in which MLP_ϕ and MLP_θ are shared across layer l.

Update operators

A simple form for the update operator would be:

$$\text{Update}(h_n^{(l)}, z_n^{(l)}) = f(W_{\text{self}} h_n^{(l)} + W_{\text{neigh}} z_n^{(l)} + b)$$

If we choose a simple summation as the aggregation function and if we also share the same weight matrix between nodes and their neighbors, we obtain a particularly simple form of the update operator:

$$h_n^{(l+1)} = \text{Update}(h_n^{(l)}, z_n^{(l)}) = f(W^{(l+1)} \sum_{m \in \mathcal{N}(n), n} h_m^{(l)} + b)$$

Node classification

We need to define a cost function for training:

- For node classification over C classes, we can use $\mathrm{softmax}(H_n^{(L)} W^{(o)})$ to output the logits, where $W^{(o)}$ is a learnable $D \times C$ matrix. The loss function is defined as the cross-entropy loss across all nodes and all classes.
- If the goal is to predict continuous values at the outputs then a simple linear transformation can be combined with a sum-of-squares error to define a suitable loss function.

Node classification

We can distinguish between three types of nodes as follows:

	$\mathcal{V}_{\text{train}}$	$\mathcal{V}_{\text{trans}}$	$\mathcal{V}_{\text{induct}}$
Labelled	Yes	No	No
Included in the message-passing operations of the graph neural network	Yes	Yes	No
Used to compute the loss function used for training	Yes	No	No

If there are no transductive nodes, then the training is generally referred to as inductive learning. However, if there are transductive nodes then it is called transductive learning.

Edge classification

A common form of edge classification task is edge completion in which the goal is to determine whether an edge should be present between two nodes. The probability $p(n, m)$ for the presence of an edge between nodes n and m can be defined as:

$$p(n, m) = \sigma(h_n^T h_m)$$

Graph classification

In some applications of graph neural networks, the goal is to predict the properties of new graphs given a training set of labelled graphs $\mathcal{G}_1, \ldots, \mathcal{G}_N$. This requires that we combine all the final-layer embedding vectors in a way that does not depend on the arbitrary node ordering:

$$y = f\left(\sum_{n \in \mathcal{V}} h_n^{(L)}\right)$$

where the function f may contain learnable parameters. Other invariant aggregation functions can be used such as averages or element-wise minimum or maximum.