An algorithmic reasoning approach to GNNs

A project for the *Deep Learning* course

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Aim of the project

Graph Neural Networks can have a lot of meanings, there isn't just one architecture that can be recognized as "GNN". We will try to understand the general, abstract structure of a GNN that is presented in the book [4] (which also includes [2]) and to shed light about the relational inductive bias and combinatorial generalization of a GNN.

Our motivation is to better understand the extent to which graph neural networks are capable of **precise and logical reasoning**.

Graph Theory

Inroduction

Graphs are a widespread data structure and a universal language for describing and modelling complex systems. In the most general view, a graph is simply a collection of objects (i.e., nodes), along with a set of interactions (i.e., edges) between pairs of these objects.

Graphs are an important building block since they can naturally encode an entity-relationship structure, as well as an invariance to permutations (of both nodes and edges) and awareness of input sparsity.

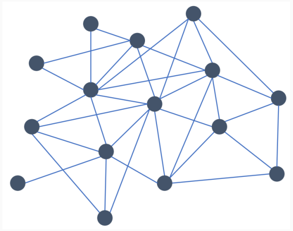


Figure 1: A graph.

Basics

Definition

A graph is a tuple $G = (V, E)$ where V is the set of nodes and E is the set of edges between these nodes. We denote an edge going from node $u \in V$ to node $v \in V$ as $(u, v) \in E$, so $E \subseteq V \times V$. The graph is **undirected** if $(u, v) \in E \iff (v, u) \in E$, otherwise it is **directed**.

Given a node u, $\mathcal{N}(u)$ is u's graph neighborhood.

A convenient way to represent graphs is through an adjacency matrix $A \in \mathbb{R}^{|V| \times |V|}$, with $A[u, v] = 1$ if $(u, v) \in E$ and $A[u, v] = 0$ otherwise. If the graph is undirected the matrix in *symmetric*. If the graph has weighted edges we have that $A[u, v] \in \mathbb{R}$.

We also have attribute or feature information associated with a graph. Most often these are *node-level attributes* that we represent using a real-valued matrix $\mathbf{X} \in \mathbb{R}^{d \times |V|}$, where we assume that the ordering of the nodes is consistent with the ordering in the adjacency matrix. In some cases we even associate real-valued *features with entire graphs*.

Machine learning on graphs

Machine learning tasks on graph data fall in one of these four categories:

- *node classification*: predict the label y_u associated with all the nodes $u \in V$
  $\longrightarrow$ E.g., predicting whether a user is a bot in a social network
- *edge prediction*: infer the edges between nodes in a graph
  $\longrightarrow$ E.g., content recommendation in online platforms, predicting drug side-effects, or inferring new facts in a relational databases
- *community detection*: infer latent community structures given only the input graph
  $\longrightarrow$ E.g., uncovering functional modules in genetic interaction networks, uncovering fraudulent groups of users in financial transaction networks
- *graph class./regr./clust.*: given a dataset of *multiple different graphs*, make independent predictions specific to each graph
  $\longrightarrow$ E.g., property prediction based on molecular graph structures

Blurring the boundaries of ML categories

At first glance, node classification appears to be a straightforward variation of standard supervised classification, but there are in fact important differences. The most important difference is that the nodes in a graph are not independent and identically distributed (i.i.d.). Usually, when we build supervised machine learning models we assume that each datapoint is statistically independent from all the other datapoints; otherwise, we might need to model the dependencies between all our input points. We also assume that the datapoints are identically distributed; otherwise, we have no way of guaranteeing that our model will generalize to new datapoints. Node classification completely breaks this i.i.d. assumption. Rather than modeling a set of i.i.d. datapoints, we are instead modeling an interconnected set of nodes.

Of all the machine learning tasks on graphs, graph regression and classification are perhaps the most straightforward analogues of standard supervised learning. Each graph is an i.i.d. datapoint associated with a label, and the goal is to use a labeled set of training points to learn a mapping from datapoints (i.e., graphs) to labels.

Node-level statistics and features

Node degree

The degree of a node $u \in V$ simply counts the number of edges incident to the node, so how many neighbors the node has:

$$d_u = \sum_{v \in V} A[u, v]. \tag{1}$$

To obtain a more powerful measure of *importance*, we can consider various measures of what is known as node centrality.

Eigenvector centrality

We define a node's eigenvector centrality e_u via a recurrence relation in which the node's centrality is proportional via a constant λ to the average centrality of its neighbors:

$$e_u = \frac{1}{\lambda} \sum_{v \in V} A[u, v] e_v \ \forall u \in V \quad \Longleftrightarrow \quad \lambda \mathbf{e} = A\mathbf{e}. \ \text{with } \mathbf{u} \text{ vector of node centralities.} \tag{2}$$

Graph-level features and graph kernels

Bag of nodes

The simplest approach to defining a graph-level feature is to just aggregate node-level statistics. For example, one can compute histograms or other summary statistics based on the degrees, centralities, and clustering coefficients of the nodes in the graph. This aggregated information can then be used as a graph-level representation. The downside to this approach is that it is entirely based upon local node-level information and can miss important global properties in the graph.

The Weisfeiler-Lehman kernel

One way to improve the basic bag of nodes approach is using a strategy of *iterative neighborhood aggregation*. The idea with these approaches is to extract node-level features that contain more information than just their local ego graph, and then to aggregate these richer features into a graph-level representation.
Perhaps the most important and well-known of these strategies is the WeisfeilerLehman (WL) algorithm and kernel.

Neighborhood Overlap Detection

The various statistical measures of neighborhood overlap between pairs of nodes quantify the extent to which a pair of nodes are related. For example, the simplest neighborhood overlap measure just counts the number of neighbors that two nodes share:

$$\mathbf{S}[u,v] = |\mathcal{N}(u) \cap \mathcal{N}(v)|, \tag{3}$$

where we use $\mathbf{S}[u,v]$ to denote the value quantifying the relationship between nodes u and v and let $\mathbf{S} \in \mathbb{R}^{|V|\times|V|}$ denote the similarity matrix summarizing all the pairwise node statistics.

Even though there is no "machine learning" involved in any of the statistical measures discussed in this section, they are still very useful and powerful baselines for relation prediction. Given a neighborhood overlap statistic $\mathbf{S}[u,v]$, a common strategy is to assume that the likelihood of an edge (u,v) is simply proportional to $\mathbf{S}[u,v]$:

$$\mathbf{P}(A[u,v]=1) \propto \mathbf{S}[u,v]. \tag{4}$$

Thus, in order to approach the relation prediction task using a neighborhood overlap measure, one simply needs to set a threshold to determine when to predict the existence

?????????

In the previous sections, we saw a number of traditional approaches to learning over graphs. However, the approaches discussed — and especially the node and graph-level statistics — are limited due to the fact that they require careful, hand-engineered statistics and measures. We will introduce an alternative approach to learning over graphs: graph representation learning. Instead of extracting hand-engineered features, we will seek to *learn* representations that encode structural information about the graph.

Neighborhood Reconstruction Methods

Frame Title

We will now see methods for learning node embeddings. The goal of these methods is to encode nodes as low-dimensional vectors that summarize their graph position and the structure of their local graph neighborhood. In other words, we want to project nodes into a latent space, where geometric relations in this latent space correspond to relationships (e.g., edges) in the original graph or network.

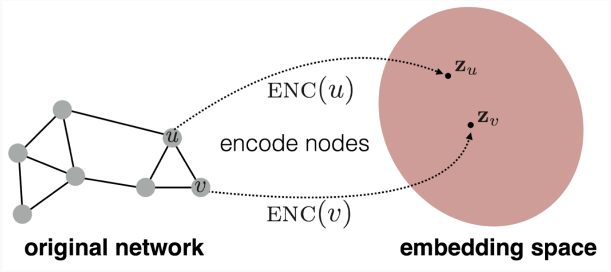
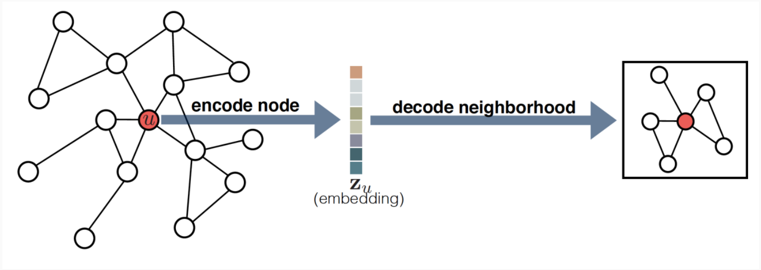


Figure 2: Illustration of the node embedding problem. Our goal is to learn an encoder (enc), which maps nodes to a low-dimensional embedding space. These embeddings are optimized so that distances in the embedding space reflect the relative positions of the nodes in the original graph.

An Encoder-Decoder Perspective

We organize our discussion of node embeddings based upon the framework of encoding and decoding graphs. In the encoder-decoder framework, we view the graph representation learning problem as involving two key operations. First, an encoder model maps each node u in the graph into a low-dimensional vector or embedding $\mathbf{z}_u$. Next, a decoder model takes the low-dimensional node embeddings $\mathbf{z}_u$ and uses them to reconstruct information about each node u's neighborhood in the original graph.



The Encoder

Formally, the encoder is a function that maps nodes $v \in V$ to vector embeddings $\mathbf{z}_v \in \mathbb{R}^d$ (where $\mathbf{z}_v$ corresponds to the embedding for node $v \in V$). In the simplest case, the encoder has the following signature:

$$\text{ENC} : V \to \mathbb{R}^d, \tag{5}$$

meaning that the encoder takes node IDs as input to generate the node embeddings. In most work on node embeddings, the encoder relies on what we call the shallow embedding approach, where this encoder function is simply an embedding lookup based on the node ID. In other words, we have that

$$\text{ENC}(v) = \mathbf{Z}[v], \tag{6}$$

where $\mathbf{Z} \in \mathbb{R}^{|V| \times d}$ is a matrix containing the embedding vectors for all nodes and $\mathbf{Z}[v]$ denotes the row of $\mathbf{Z}$ corresponding to node v.

The Decoder

The role of the decoder is to reconstruct certain graph statistics from the node embeddings that are generated by the encoder. For example, given a node embedding $\mathbf{z}_u$ of a node u, the decoder might attempt to predict u's set of neighbors $\mathcal{N}(u)$ or its row $A[u]$ in the graph adjacency matrix.

While many decoders are possible, the standard practice is to define pairwise decoders, which have the following signature:

$$\text{DEC} : \mathbb{R}^d \times \mathbb{R}^d \to \mathbb{R}^+. \tag{7}$$

Pairwise decoders can be interpreted as predicting the relationship or similarity between pairs of nodes. For instance, a simple pairwise decoder could predict whether two nodes are neighbors in the graph.

Applying the pairwise decoder to a pair of embeddings $(\mathbf{z}_u, \mathbf{z}_v)$ results in the *reconstruction* of the relationship between nodes u and v. The goal is optimize the encoder and decoder to minimize the reconstruction loss so that

$$\text{DEC}(\text{ENC}(u), \text{ENC}(v)) = \text{DEC}(\mathbf{z}_u, \mathbf{z}_v) \approx \mathbf{S}[u, v]. \tag{8}$$

Optimizing an Encoder-Decoder Model

To achieve the reconstruction objective (8), the standard practice is to minimize an empirical reconstruction loss $\mathcal{L}$ over a set of training node pairs $\mathcal{D}$:

$$\mathcal{L} = \sum_{(u,v)\in\mathcal{D}} \ell(\text{DEC}(\mathbf{z}_u, \mathbf{z}_v), \mathbf{S}[u, v]), \tag{9}$$

where $\ell : \mathbb{R} \times \mathbb{R} \to \mathbb{R}$ is a loss function measuring the discrepancy between the decoded (i.e., estimated) similarity values $\text{DEC}(\mathbf{z}_u, \mathbf{z}_v)$ and the true values $\mathbf{S}[u, v]$. Depending on the definition of the decoder (DEC) and similarity function ($\mathbf{S}$), the loss function ℓ might be a mean-squared error or even a classification loss, such as cross entropy. Thus, the overall objective is to train the encoder and the decoder so that pairwise node relationships can be effectively reconstructed on the training set $\mathcal{D}$. Most approaches minimize the loss in 9 using stochastic gradient descent, but there are certain instances when more specialized optimization methods (e.g., based on matrix factorization) can be used.

Limitations of Shallow Embeddings

This focus of this chapter has been on shallow embedding methods. In these approaches, the encoder model that maps nodes to embeddings is simply an embedding lookup (6), which trains a unique embedding for each node in the graph. However, it is also important to note that shallow embedding approaches suffer from some important drawbacks:

- The first issue is that they do not share any parameters between nodes in the encoder, since the encoder directly optimizes a unique embedding vector for each node. This lack of parameter sharing is both statistically and computationally inefficient.
- A second key issue is that they do not leverage node features in the encoder.
- Lastly — and perhaps most importantly — they are inherently *transductive*. These methods can only generate embeddings for nodes that were present during the training phase. Generating embeddings for new nodes — which are observed after the training phase — is not possible unless additional optimizations are performed to learn the embeddings for these nodes. This restriction prevents shallow embedding methods from being used on *inductive* applications, which involve

The Graph Neural Network Model

A stupid GNN

To define a deep neural network over graphs one could simply use the adjacency matrix as input to a deep neural network. For example, to generate an embedding of an entire graph we could simply flatten the adjacency matrix and feed the result to a multi-layer perceptron (MLP):

$$\mathbf{z}_G = \text{MLP}(\mathbf{A}[1] \oplus \mathbf{A}[2] \oplus \ldots \oplus \mathbf{A}[|\mathcal{V}|]); \tag{10}$$

where $\mathbf{A}[i] \in \mathbf{R}^{|\mathcal{V}|}$ denotes a row of the adjacency matrix and we use $\oplus$ to denote vector concatenation.

The issue with this approach is that it *depends on the arbitrary ordering of nodes that we used in the adjacency matrix*. In other words, such a model is not permutation invariant.

Any function f that takes an adjacency matrix $\mathbf{A}$ as input should ideally satisfy one of the two following properties, given a permutation matrix $\mathbf{P}$:

$$f(\mathbf{PAP}^T) = f(\mathbf{A}) \qquad \text{(Permutation Invariance)} \tag{11}$$

$$f(\mathbf{PAP}^T) = \mathbf{P}f(\mathbf{A}) \qquad \text{(Permutation Equivariance),} \tag{12}$$

Neural Message Passing

How we can take an input graph $G = (V, E)$, along with a set of node features $\mathbf{X} \in \mathbb{R}^{d \times |V|}$, and use this information to generate node embeddings $\mathbf{z}_u, \forall u \in V$?

During each message-passing iteration k in a GNN, a hidden embedding $\mathbf{h}_u^{(k)}$ corresponding to each node $u \in \mathcal{V}$ is updated according to information aggregated from u's graph neighborhood $\mathcal{N}(u)$. This message-passing update can be expressed as follows:

$$\mathbf{h}_u^{(k+1)} = \text{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}; \text{AGGREGATE}^{(k)}(\{\mathbf{h}_v^{(k)}, \forall v \in \mathcal{N}(u)\})\right) \tag{13}$$

$$= \text{UPDATE}^{(k)}\left(\mathbf{h}_u^{(k)}, \mathbf{m}_{\mathcal{N}(u)}^{(k)}\right), \tag{14}$$

where UPDATE and AGGREGATE are arbitrary differentiable functions (i.e., neural networks) and $\mathbf{m}_{\mathcal{N}(u)} = \text{AGGREGATE}(\{\mathbf{h}_v, \forall v \in \mathcal{N}(u)\})$ is the "message" that is aggregated from u's graph neighborhood $\mathcal{N}(u)$ (neighborhood aggregation operation). The different iterations of message passing are also sometimes known as the different "layers" of the GNN.

Message Passing in Practice

The initial embeddings at k = 0 are set to the input features for all the nodes, i.e., $\mathbf{h}_u^{(0)} = \mathbf{x}_u, \forall u \in \mathcal{V}$. After running K iterations of the GNN message passing, we can use the output of the final layer to define the embeddings for each node, i.e.,

$$\mathbf{z}_u = \mathbf{h}_u^{(K)}, \forall u \in \mathcal{V}. \tag{15}$$

Note that since the AGGREGATE function takes a set as input, GNNs defined in this way are permutation equivariant by design.

Basic intuition $\longrightarrow$ at each iteration, every node aggregates information from its local neighborhood, and as these iterations progress each node embedding contains more and more information from further reaches of the graph.

- *structural information* about the graph $\longrightarrow$ after k iterations, $\mathbf{h}_u^{(k)}$ might encode information about the degrees of all the nodes in u's k-hop neighborhood.
- *feature-based information* about the graph $\longrightarrow$ after k iterations, $\mathbf{h}_u^{(k)}$ also encodes information about all the features in its k-hop neighborhood $\rightarrow$ analogous to convolutional kernels in CNNs!

The Basic GNN

The basic GNN message passing is defined as

$$\mathbf{h}_u^{(k)} = \sigma\left(\mathbf{W}_{\text{self}}^{(k)}\mathbf{h}_u^{(k-1)} + \mathbf{W}_{\text{neigh}}^{(k)}\sum_{v\in\mathcal{N}(u)}\mathbf{h}_v^{(k-1)} + \mathbf{b}^{(k)}\right), \tag{16}$$

where $\mathbf{W}_{\text{self}}^{(k)}, \mathbf{W}_{\text{neigh}}^{(k)} \in \mathbb{R}^{d^{(k)}\times d^{(k-1)}}$ are trainable parameter matrices and σ denotes an elementwise non-linearity (e.g., a tanh or ReLU). The bias term $b^{(k)} \in \mathbb{R}^{d^{(k)}}$ is often omitted for notational simplicity, but including it can be important to achieve strong performance.

We can equivalently define the basic GNN through the UPDATE and AGGREGATE functions:

$$\mathbf{m}_{\mathcal{N}(u)} = \sum_{v\in\mathcal{N}(u)}\mathbf{h}_v, \tag{17}$$

$$\text{UPDATE}(\mathbf{h}_u, \mathbf{m}_{\mathcal{N}(u)}) = \sigma\left(\mathbf{W}_{\text{self}}\mathbf{h}_u + \mathbf{W}_{\text{neigh}}\mathbf{m}_{\mathcal{N}(u)}\right), \tag{18}$$

Any GNNs can also be succinctly defined using graph-level equations. In the case of a basic GNN, we can write the graph-level definition of the model as follows:

Message Passing with Self-loops

As a simplification of the neural message passing approach, it is common to add self-loops to the input graph and omit the explicit update step. In this approach we define the message passing simply as

$$\mathbf{h}_u^{(k)} = \text{AGGREGATE}(\{\mathbf{h}_v^{(k-1)}, \forall v \in \mathcal{N}(u) \cup \{u\}\}), \tag{20}$$

where now the aggregation is taken over the set $\mathcal{N}(u) \cup \{u\}$, i.e., the node's neighbors as well as the node itself. The benefit of this approach is that we no longer need to define an explicit update function, as the update is implicitly defined through the aggregation method.

In the case of the basic GNN, adding self-loops is equivalent to sharing parameters between the $\mathbf{W}_{\text{self}}$ and $\mathbf{W}_{\text{neigh}}$ matrices, which gives the following graph-level update:

$$\mathbf{H}^{(k)} = \sigma\left((A + I)\mathbf{H}^{(k-1)}\mathbf{W}^{(k)}\right). \tag{21}$$

In the following chapters we will refer to this as the self-loop approach.

Graph convolutional networks (GCNs)

The most basic neighborhood aggregation operation (17) simply takes the sum of the neighbor embeddings. One issue with this approach is that it can be unstable and highly sensitive to node degrees. One solution to this problem is to simply *normalize the aggregation operation* based upon the degrees of the nodes involved:

$$\mathbf{m}_{\mathcal{N}(u)} = \frac{\sum_{v \in \mathcal{N}(u)} \mathbf{h}_v}{|\mathcal{N}(u)|}. \tag{22}$$

Another normalization factor is the symmetric normalization:

$$\mathbf{m}_{\mathcal{N}(u)} = \sum_{v \in \mathcal{N}(u)} \frac{\mathbf{h}_v}{\sqrt{|\mathcal{N}(u)||\mathcal{N}(v)|}}. \tag{23}$$

The popular graph convolutional network (GCN) employs the *symmetric-normalized aggregation* as well as the *self-loop approach*, using as message passing function

$$h_u^{(k)} = \sigma\left(\mathbf{W}^{(k)} \sum_{v \in \mathcal{N}(u) \cup \{u\}} \frac{\mathbf{h}_v}{\sqrt{|\mathcal{N}(u)||\mathcal{N}(v)|}}\right). \tag{24}$$

Improving the Aggregation Layer

An aggregation function with the following form is a universal set function approximator:

$$\mathbf{m}_{\mathcal{N}(u)} = \text{MLP}_\theta\left(\sum_{v\in\mathcal{N}(u)} \text{MLP}_\phi(\mathbf{h}_v)\right). \tag{25}$$

So any permutation-invariant function that maps a set of embeddings to a single embedding can be approximated to an arbitrary accuracy by a model following (25).
$\longrightarrow$ set pooling leads small increases in performance but increased risk of overfitting

Another strategy is to apply attention: assign an attention weight or importance to each neighbor, which is used to weigh this neighbor's influence during the aggregation step. The first GNN model to apply this style of attention was the Graph Attention Network (GAT):

$$\mathbf{m}_{\mathcal{N}(u)} = \sum_{v\in\mathcal{N}(u)} \alpha_{u,v}\mathbf{h}_v, \tag{26}$$

where $\alpha_{u,v}$ denotes the attention on neighbor $v \in \mathcal{N}(u)$ (*neighborhood attention*) when we are aggregating information at node u.

Visualize a single GAT step

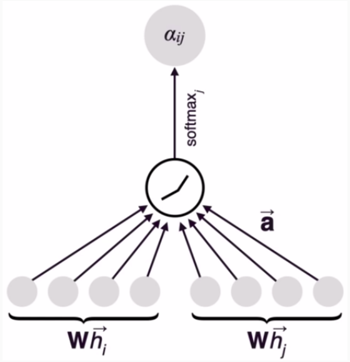


Figure 3: Attention mechanism. It looks at features of node i and its neighbor j, then the attention function computes the coefficient α_{ij}, which signifies the influence of node i to node j.

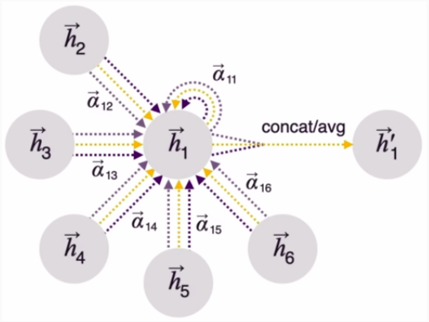


Figure 4: Multi-head attention mechanism. Each colored line indicates a different way in which the node receives information from its immediate neighbors, which is aggregated to produce an updated representation.

Images from [8]

Graph Pooling

What if we want to learn an embedding $\mathbf{z}_G$ for the entire graph G? $\longrightarrow$ graph pooling

We want to design a pooling function f_p, which maps a set of node embeddings $\{\mathbf{z}_1, \dots, \mathbf{z}_{|V|}\}$ to an embedding $\mathbf{z}_G$ that represents the full graph.

One approach is to simply to take a sum (or mean) of the node embeddings:

$$\mathbf{z}_G = \frac{\sum_{v \in V} \mathbf{z}_u}{f_n(|V|)}, \tag{27}$$

where f_n is some normalizing function (e.g., the identity function, so $\mathbf{z}_G = (\sum_{v \in V} \mathbf{z}_u)/|V|$).

Limitation: it does not exploit the structure of the graph! We want to exploit the graph topology at the pooling stage. $\longrightarrow$ use graph clustering or coarsening

Generalized Message Passing

The presentation in this chapter so far has focused on the most popular style of GNN message passing, which operates largely at the node level. However, the GNN message passing approach can also be generalized to leverage edge and graph-level information at each stage of message passing. For example, in the more general approach proposed by [2], we define each iteration of message passing according to the following equations:

$$\mathbf{h}_{(u,v)}^{(k)} = \text{UPDATE}_{\text{edge}}(\mathbf{h}_{(u,v)}^{(k-1)}, \mathbf{h}_{u}^{(k-1)}, \mathbf{h}_{v}^{(k-1)}, \mathbf{h}_{G}^{(k-1)}) \tag{28}$$

$$\mathbf{m}_{\mathcal{N}(u)} = \text{AGGREGATE}_{\text{node}}(\{\mathbf{h}_{(u,v)}^{(k)}, \ \forall v \in \mathcal{N}(u)\}) \tag{29}$$

$$\mathbf{h}_{u}^{(k)} = \text{UPDATE}_{\text{node}}(\mathbf{h}_{u}^{(k-1)}, \mathbf{m}_{\mathcal{N}(u)}, \mathbf{h}_{G}^{(k-1)}) \tag{30}$$

$$\mathbf{h}_{G}^{(k)} = \text{UPDATE}_{\text{graph}}(\mathbf{h}_{G}^{(k-1)}, \{\mathbf{h}_{u}^{(k)}, \ \forall u \in V\}, \{\mathbf{h}_{(u,v)}^{(k)}, \forall (u,v) \in E\}). \tag{31}$$

The important innovation in this generalized message passing framework is that, during message passing, we generate hidden embeddings $\mathbf{h}_{(u,v)}^{(k)}$ for each edge in the graph, as well as an embedding $h_{G}^{(k)}$ corresponding to the entire graph. This allows the message passing model to easily integrate edge and graph-level features, and recent work has also shown this generalized message passing approach to have benefits compared to a

Graph Neural Networks in Practice i

In the vast majority of current applications, GNNs are used for one of three tasks: node classification, graph classification, or relation prediction.

- *GNNs for Node Classification* $\rightarrow$ train GNNs in a fully-supervised manner with a negative log-likelihood loss:

$$\mathcal{L} = \sum_{u \in V_{\text{train}}} -\log(\text{softmax}(\mathbf{z}_u, \mathbf{y}_u)), \tag{32}$$

where $\mathbf{y}_u$ is a one-hot vector indicating the class of training node $u \in V_{\text{train}}$ and $\text{softmax}(\mathbf{z}_u, \mathbf{y}_u)$ denotes the predicted probability that the node belongs to the class $\mathbf{y}_u$, computed via the softmax function:

$$\text{softmax}(\mathbf{z}_u, \mathbf{y}_u) = \sum_{i=1}^{c} \mathbf{y}_u[i] \frac{e^{\mathbf{z}_u^\top \mathbf{w}_i}}{\sum_{j=1}^{c} e^{\mathbf{z}_u^\top \mathbf{w}_j}}, \tag{33}$$

Graph Neural Networks in Practice ii

where $\mathbf{w}_i \in \mathbb{R}^d, i = 1, \ldots, c$ are trainable parameters.

- *GNNs for Graph Classification* $\rightarrow$ a softmax classification loss — analogous to 33 — is often used, with the key difference that the loss is computed with graph-level embeddings $\mathbf{z}_{G_i}$ over a set of labeled training graphs $\mathcal{G} = \{G_1, \ldots, G_n\}$. In recent years, GNNs have also witnessed success in regression tasks involving graph data. In these instances, it is standard to employ a squared-error loss of the following form:

$$\mathcal{L} = \sum_{G_i \in \mathcal{G}} \|\mathsf{MLP}(\mathbf{z}_{G_i}) - y_{G_i}\|_2^2, \tag{34}$$

where **MLP** is a densely connected neural network with a univariate output and $y_{G_i} \in \mathbb{R}$ is the target value for training graph G_i.

Graph Neural Networks in Practice iii

- *GNNs for Edge Prediction* $\rightarrow$ While classification tasks are by far the most popular application of GNNs, GNNs are also used in in edge prediction tasks, such as recommender systems and knowledge graph completion. In these applications, the standard practice is to employ the pairwise node embedding loss functions. In principle, GNNs can be combined with any of the pairwise loss functions discussed previously, with the output of the GNNs replacing the shallow embeddings.

Relational inductive biases in graph networks

Our GN framework imposes several strong relational inductive biases when used as components in a learning process. First, graphs can express arbitrary relationships among entities, which means the GN's input determines how representations interact and are isolated, rather than those choices being determined by the fixed architecture. For example, the assumption that two entities have a relationship—and thus should interact—is expressed by an edge between the entities' corresponding nodes. Similarly, the absence of an edge expresses the assumption that the nodes have no relationship and should not influence each other directly.

Second, graphs represent entities and their relations as sets, which are invariant to permutations. This means GNs are invariant to the order of these elements[1], which is often desirable. For example, the objects in a scene do not have a natural ordering (see Sec. **??**).

Third, a GN's per-edge and per-node functions are reused across all edges and nodes, respectively. This means GNs automatically support a form of combinatorial generalization (see Section **??**): because graphs are composed of edges, nodes, and

Combinatorial Optimization and Reasoning with GNN

Thank you for your attention!

☺

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