FACULDADE DE CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA

Graph Neural Networks

Rui Valente de Almeida

April 30, 2019

FCT NOVA

FACULDADE DE CIÊNCIAS E TECNOLOGIA
UNIVERSIDADE NOVA DE LISBOA
Graph Neural Networks
Rui Valente de Almeida
April 30, 2019
FCT NOVA

Structure

This presentation was done as one of the assignments for the ISM PhD course. It is focused around Graph Neural Networks, on the theoretical and practical side.

Most of the presentation was built using two articles:

- Zonham et al.: *A comprehensive survey on Graph Neural Networks*;
- Zhou et al.: *Graph Neural Networks: a review of methods and applications*

Test 2

Structure

This presentation was done as one of the assignments for the ISM PhD course. It is focused around Graph Neural Networks, on the theoretical and practical side.

Most of the presentation was built using two articles:

- Zonham et al.: *A comprehensive survey on Graph Neural Networks*;
- Zhou et al.: *Graph Neural Networks: a review of methods and applications*

Structure

The presentation is structured as follows:

- Theoretical background: graphs, Artificial Neural Networks and Graph Neural Networks;
- GNN applications;
- Conclusions.

Structure

The presentation is structured as follows:

- Theoretical background: graphs, Artificial Neural Networks and Graph Neural Networks;
- GNN applications;
- Conclusions.

Graphs

A graph is an ordered pair (V(G), E(G)) and an incidence function ψ_G

Graphs
A graph is an ordered pair (V(G), E(G)) and an incidence function ψ_G

Graphs

A graph is an ordered pair (V(G), E(G)) and an incidence function ψ_G

- V(G) is the set of vertices (or nodes);
- E(G) is the set of edges;

Graphs
A graph is an ordered pair (V(G), E(G)) and an incidence function ψ_G
- V(G) is the set of vertices (or nodes);
- E(G) is the set of edges;

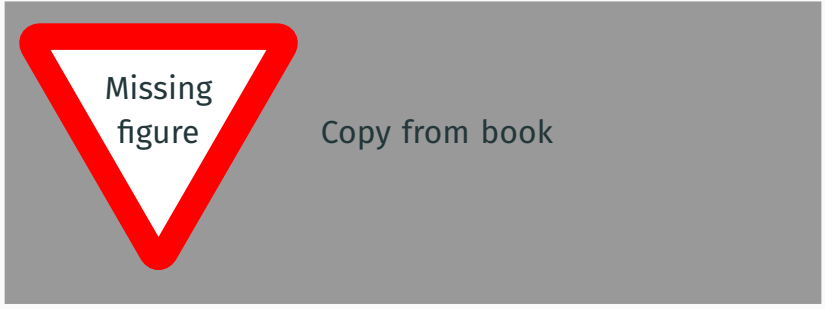
Graphs

The incidence functions creates relations between V and E. Let $e \in E$ and $u, v \in V$. Then if $\psi_G(e) = uv$, e is said to join u and v.

Graphs
The incidence functions creates relations between V and E. Let $e \in E$ and $u, v \in V$. Then if $\psi_G(e) = uv$, e is said to join u and v.

Defining a Graph

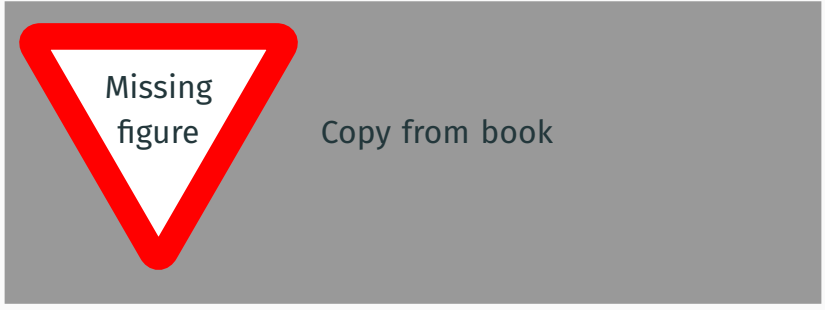
We can use a purely mathematical (analytical) form to write a graph:



Defining a Graph
We can use a purely mathematical (analytical) form to write a graph:
Missing figure
Copy from book

Defining a Graph

Sure it is rigorous, but also cumbersome!



Defining a Graph
Sure it is rigorous, but also cumbersome!
Missing figure
Copy from book

Defining a Graph

Copy graph nottaion

- Nodes are represented by a dot (may or not be filled);
- Edges are represented by lines.
- Vertices positions and line curve are usually non-significant.

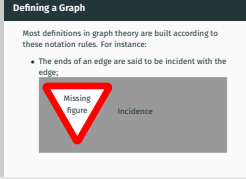
Defining a Graph
Missing figure
Copy graph nottaion
- Nodes are represented by a dot (may or not be filled);
- Edges are represented by lines.
- Vertices positions and line curve are usually non-significant.

- Nodes can also be represented by vectors of features;
- When this representation is chosen, we can then write all the nodes as a matrix of features

Defining a Graph

Most definitions in graph theory are built according to these notation rules. For instance:

- The ends of an edge are said to be incident with the edge;



Defining a Graph

- Two vertices that are incident with the same edge are adjacent, as are two edges that are incident with the same vertex;

Defining a Graph
- Two vertices that are incident with the same edge are adjacent, as are two edges that are incident with the same vertex;
Missing figure
Adjacency

Defining a Graph

- Two distinct adjacent vertices are called neighbours. The set of neighbours of vertex v in graph G is denoted $N_G(v)$.

Defining a Graph
• Two distinct adjacent vertices are called neighbours. The set of neighbours of vertex v in graph G is denoted $N_G(v)$.
Missing figure
Neighbours

Graph digital representation

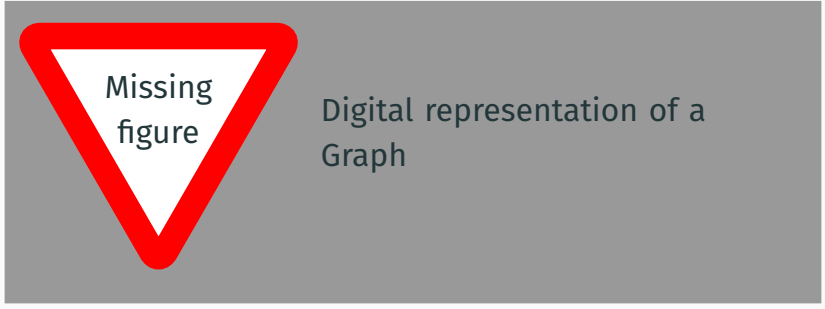
As humans, we prefer graphical representations (an image is worth a thousand words). This is useless for a computer!

Graph digital representation
As humans, we prefer graphical representations (an image is worth a thousand words). This is useless for a computer!

Graph digital representation

As humans, we prefer graphical representations (an image is worth a thousand words). This is useless for a computer!

But we can also represent a graph in matricial form:



Digital representation of a Graph

Graph digital representation
As humans, we prefer graphical representations (an image is worth a thousand words). This is useless for a computer!
But we can also represent a graph in matricial form:
Missing figure
Digital representation of a Graph

Graph digital representation

Let $\boldsymbol{M}_G \in \mathbb{R}^{m \times n}$ be the incidence matrix of G. Then $\boldsymbol{M}_G := (m_{ve})$, where m_{ve} is the number of times (0, 1 or 2) that vertex v and edge e are incident.

Graph digital representation
Let $\boldsymbol{M}_G \in \mathbb{R}^{m \times n}$ be the incidence matrix of G. Then $\boldsymbol{M}_G := (m_{ve})$, where m_{ve} is the number of times (0, 1 or 2) that vertex v and edge e are incident.

Graph digital representation

Let $\boldsymbol{M}_G \in \mathbb{R}^{m \times n}$ be the incidence matrix of G. Then $\boldsymbol{M}_G := (m_{ve})$, where m_{ve} is the number of times (0, 1 or 2) that vertex v and edge e are incident.

Let $\boldsymbol{A}_G \in \mathbb{R}^{n \times n}$ be the adjacency matrix of G. Then $\boldsymbol{A}_G := (a_{uv})$, where a_{uv} is the number of edges joining vertices u and v.

Graph digital representation
Let $\boldsymbol{M}_G \in \mathbb{R}^{m \times n}$ be the incidence matrix of G. Then $\boldsymbol{M}_G := (m_{ve})$, where m_{ve} is the number of times (0, 1 or 2) that vertex v and edge e are incident.
Let $\boldsymbol{A}_G \in \mathbb{R}^{n \times n}$ be the adjacency matrix of G. Then $\boldsymbol{A}_G := (a_{uv})$, where a_{uv} is the number of edges joining vertices u and v.

There are other, more compact, versions of digital representatin of graphs. This falls out of the scope of this presentation.

Graph Signal Processing

As long as it's undirected, a graph can be represented by its normalised Laplacian matrix:

$$\boldsymbol{L}^{sym} = \boldsymbol{I}_n - \boldsymbol{D}^{-\frac{1}{2}}\boldsymbol{A}\boldsymbol{D}^{-\frac{1}{2}}$$

In this equation, $\boldsymbol{A}$ is the adjacency matrix and $\boldsymbol{D}$ is a diagonal matrix of node degrees, $\boldsymbol{D}_{ii} = \sum_j (A_{ij})$.

Graph Signal Processing

As long as it's undirected, a graph can be represented by its normalised Laplacian matrix:

$$\boldsymbol{L}^{sym} = \boldsymbol{I}_n - \boldsymbol{D}^{-\frac{1}{2}}\boldsymbol{A}\boldsymbol{D}^{-\frac{1}{2}}$$

In this equation, $\boldsymbol{A}$ is the adjacency matrix and $\boldsymbol{D}$ is a diagonal matrix of node degrees, $\boldsymbol{D}_{ii} = \sum_j (A_{ij})$.

- An undirected graph is one for which the edges have no particular direction.

Graph Signal Processing

This matrix is real symmetric positive semidefinite, so it can be factorised as:

$$\boldsymbol{L}^{sym} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$$

Where $\boldsymbol{U} = [\boldsymbol{u}_0, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_{n-1}] \in \mathbb{R}^N$ is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues, $\Lambda_{ii} = \lambda_i$

Graph Signal Processing
This matrix is real symmetric positive semidefinite, so it can be factorised as:
$\boldsymbol{L}^{sym} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^T$
Where $\boldsymbol{U} = [\boldsymbol{u}_0, \boldsymbol{u}_1, \ldots, \boldsymbol{u}_{n-1}] \in \mathbb{R}^N$ is the matrix of eigenvectors and Λ is the diagonal matrix of eigenvalues, $\Lambda_{ii} = \lambda_i$

- To this we call the eigendecomposition
- $\boldsymbol{U}^T\boldsymbol{U} = \boldsymbol{I}$

Graph Signal Processing

A graph signal is denoted $\boldsymbol{x} \in \mathbb{R}^N$, with $\boldsymbol{x}_i$ being the value of the i^{th} node.

Graph Signal Processing
A graph signal is denoted $\boldsymbol{x} \in \mathbb{R}^N$, with $\boldsymbol{x}_i$ being the value of the i^{th} node.

- It's like if a node is in fact a vector.

Graph Signal Processing

A graph signal is denoted $\boldsymbol{x} \in \mathbb{R}^N$, with $\boldsymbol{x}_i$ being the value of the i^{th} node.

The graph's signal Fourier transform is written $\mathcal{F}(\boldsymbol{x}) = \boldsymbol{U}^T\boldsymbol{x}$, with the inverse being $\mathcal{F}^{-1}(\hat{\boldsymbol{x}}) = U\hat{\boldsymbol{x}}$, with $\hat{\boldsymbol{x}}$ being the transformed signal.

- It's like if a node is in fact a vector.

Graph Signal Processing
A graph signal is denoted $\boldsymbol{x} \in \mathbb{R}^N$, with $\boldsymbol{x}_i$ being the value of the i^{th} node.
The graph's signal Fourier transform is written $\mathcal{F}(\boldsymbol{x}) = \boldsymbol{U}^T\boldsymbol{x}$, with the inverse being $\mathcal{F}^{-1}(\hat{\boldsymbol{x}}) = U\hat{\boldsymbol{x}}$, with $\hat{\boldsymbol{x}}$ being the transformed signal.

Graph Convolution

It is usually easier to perform a convolution in the Fourier space. In it, the convolution operation maps to a multiplication. We can thus write of the convolution of a graph with a filter $\boldsymbol{g}$:

$$\boldsymbol{x} \star \boldsymbol{g} = \mathcal{F}^{-1}\left(\mathcal{F}\left(\boldsymbol{x}\right) \odot \mathcal{F}\left(\boldsymbol{g}\right)\right)$$

Where $\odot$ denotes element-wise product (instead of matrix product).

Graph Convolution
It is usually easier to perform a convolution in the Fourier space. In it, the convolution operation maps to a multiplication. We can thus write of the convolution of a graph with a filter $\boldsymbol{g}$:
$\boldsymbol{x} \star \boldsymbol{g} = \mathcal{F}^{-1}\left(\mathcal{F}\left(\boldsymbol{x}\right) \odot \mathcal{F}\left(\boldsymbol{g}\right)\right)$
Where $\odot$ denotes element-wise product (instead of matrix product).

Graph Convolution

Now, the previous equation can be decomposed with the Fourier transform definition for graph signals:

$$\boldsymbol{x} \star \boldsymbol{g} = \boldsymbol{U} \left(\boldsymbol{U}^T \boldsymbol{x} \odot \boldsymbol{U}^T \boldsymbol{g} \right)$$

This considering $\boldsymbol{g} \in \mathbb{R}^N$ as a signal itself, which it is.

Graph Convolution

Now, the previous equation can be decomposed with the Fourier transform definition for graph signals:

$$\boldsymbol{x} \star \boldsymbol{g} = \boldsymbol{U} \left(\boldsymbol{U}^T \boldsymbol{x} \odot \boldsymbol{U}^T \boldsymbol{g} \right)$$

This considering $\boldsymbol{g} \in \mathbb{R}^N$ as a signal itself, which it is.

This is the definition of convolution that is used in both papers and in the GNN community at large, as far as I had the opportunity to see.

This definition of convolution has a problem: is is computationally very heavy and many times prohibitively so. To circumvent this problem, some authors have suggested using polynomial expansions, such as Chebyshev's, to represent the matrices

Artificial Neural Networks

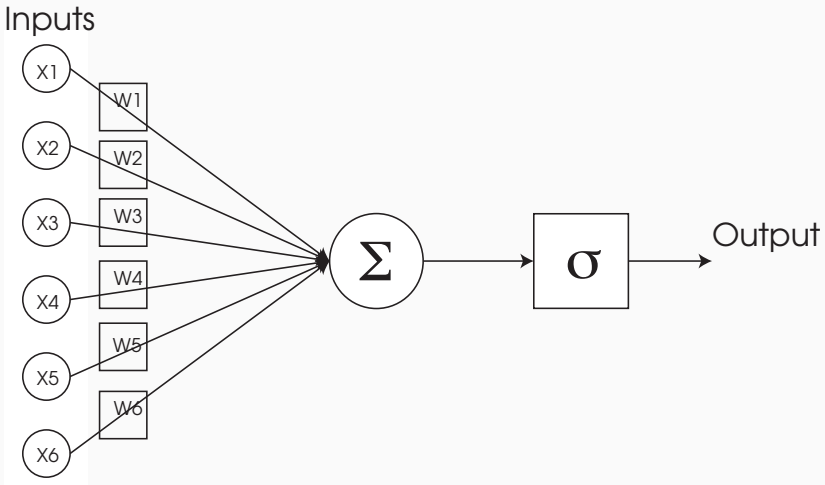
Artificial Neural Networks are today's most popular artificial intelligence tools.

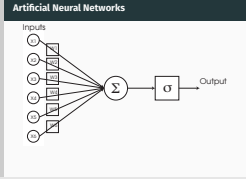
Artificial Neural Networks

Artificial Neural Networks are today's most popular artificial intelligence tools.

For all the misticism around them, ANNs are remarkably simple mathematical entities, especially given the fact that they are (really) capable of solving any problem that can be expressed as a function.

Artificial Neural Networks





- ANNs stem from mathematical theories developed in the 1940s;
- The most basic form of modern ANN, the perceptron, was created in the 1950s;
- Back then, the structure had some problems, namely the fact that it could not compute the exclusive-or operation.
- Everything changed in the 1980s, when the backpropagation algorithm was invented.

Artificial Neural Networks

The backpropagation algorithm appeared in the 1980's:

$$W^{t+1} = W^t - \eta \nabla_E^t$$

In which t is hte iteration, W represents the weights, η the learning rate and ∇_E the gradient of the loss function (which normally is MSE).

Artificial Neural Networks

The backpropagation algorithm appeared in the 1980's:

$W^{t+1} = W^t - \eta \nabla_E^t$

In which t is hte iteration, W represents the weights, η the learning rate and ∇_E the gradient of the loss function (which normally is MSE).

- First models of neural network could not implement the exclusive-or;
- For that, and for the comuptational cost, they were less used than they promised;

Artificial Neural Networks

The backpropagation algorithm appeared in the 1980's:

$$W^{t+1} = W^t - \eta \nabla_E^t$$

In which t is hte iteration, W represents the weights, η the learning rate and ∇_E the gradient of the loss function (which normally is MSE).

Artificial Neural Networks
The backpropagation algorithm appeared in the 1980's:
$W^{t+1} = W^t - \eta \nabla_E^t$
In which t is hte iteration, W represents the weights, η the learning rate and ∇_E the gradient of the loss function (which normally is MSE).

- gradient descent is used to minimize the loss function;
- the learning rate parameterises GD so that we can escape or avoid local minima;
- with this algorithm, and the introduction of non-linearities like the sigmoid or the ReLu functions in the network, ANNs can literally approximate any function.

Artificial Neural Networks

Michael Nielse has a very good interactive explanation for the Universal Approximation Theorem.

Michael Nielsen's Universal Approximation Theorem graphical demonstration

Artificial Neural Networks

Michael Nielse has a very good interactive explanation for the Universal Approximation Theorem.

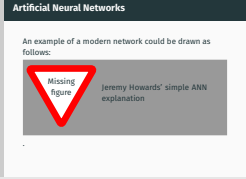
Missing figure

Michael Nielsen's Universal Approximation Theorem graphical demonstration

Artificial Neural Networks

An example of a modern network could be drawn as follows:

.



- ANNS are just a stack of linear and non linear operations that can approximate any problem in function form to any precision;
- They rely on simple matrix operations, like multiplication and convolution

Graph Neural Networks

Graphs are data just like any other...but they are non Euclidean!

Graph Neural Networks
Graphs are data just like any other...but they are non Euclidean!

- In Euclidean data, spatial structure is well and hard defined;
- We always know the distance between one ”node” and the next;
- in graphs and non-euclidean data, this is not true –it is highly irregular
- So if we want to classify graphs..how do we do it?

Graph Neural Networks

The first attempts were based on the RNN approach

Graph Neural Networks
The first attempts were based on the RNN approach
Missing figure
Microsoft presentation slide

- Consider a feature vector for each node;
- Consider each feature as a message (remember envelope);
- Each ”message” is passed to the next iteration order neighbour of every node;
- In the end, messages are summed and classified;

Graph Neural Networks

The first attempts were based on the RNN approach

Graph Neural Networks
The first attempts were based on the RNN approach
Missing figure
Microsoft presentation slide

- In this model, information decays too rapidly with node distance (exponential deacy)
- Next models were Gated Recurrent Units, which addressed this deacying problem
- In the mean time, some models appeared which instead of RNNs, were based in convolution and CNN approach.
- In fact, Gilmer et al claim that GCNs and GRNN are the same thing, and generalise it using two operating moments;

Graph Convolutional Networks

Besides RNN methods, the community has also worked on generalising CNN methods to work with graphs. The results are Graph Convolutional Networks.

Graph Convolutional Networks
Besides RNN methods, the community has also worked on generalising CNN methods to work with graphs. The results are Graph Convolutional Networks.

Graph Convolutional Networks

There are two main families of GCN:

- Spectral based;
- Spatial based;

Graph Convolutional Networks
There are two main families of GCN:
- Spectral based;
- Spatial based;

- Spectral based systems introduce filters as in graph signal Processing
- Spatial based systems see convolutions as aggregating feature information from neighbours.
- The first types of GNN were spatial based GCN
- In 2016, a paper appeared which generalises both types of GNN, with a method called Message passing graph neural networks;

Applications of GNNS

Applications

There are already many applications of this recent field of study.

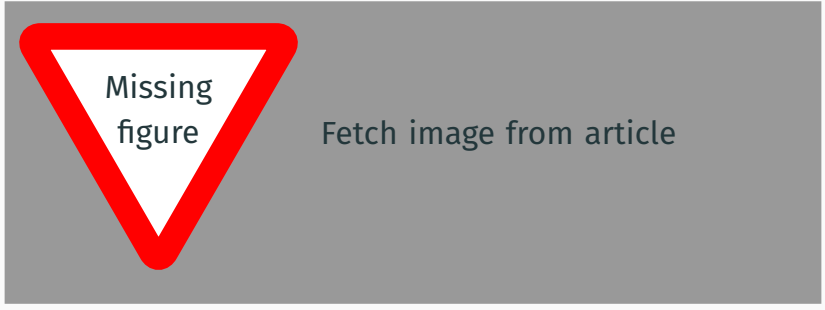
Social Network relationship analysis

Applications
There are already many applications of this recent field of study.
Missing figure
Social Network relationship analysis

- text;
- image classification;
- Social relationship analysis;
- Semantic segmentation;
- We present some of the main applications of AI in graphs;

Applications

Physical Systems simulation;

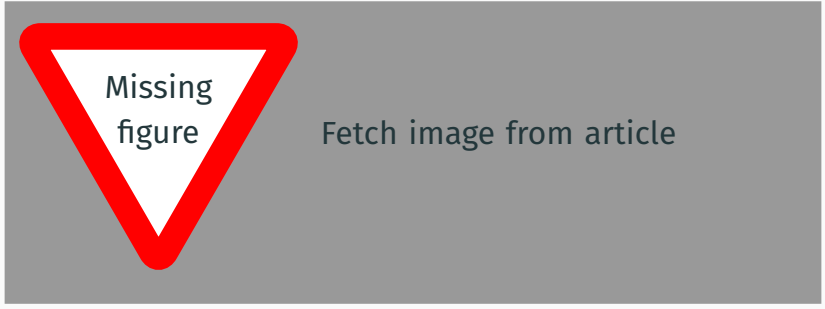


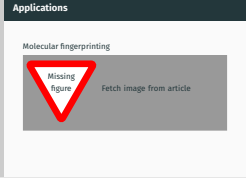
Applications
Physical Systems simulation;
Missing figure
Fetch image from article

- This system was developed in x and Y;
- It tries to simulate and predict interactions between physical bodies;
-

Applications

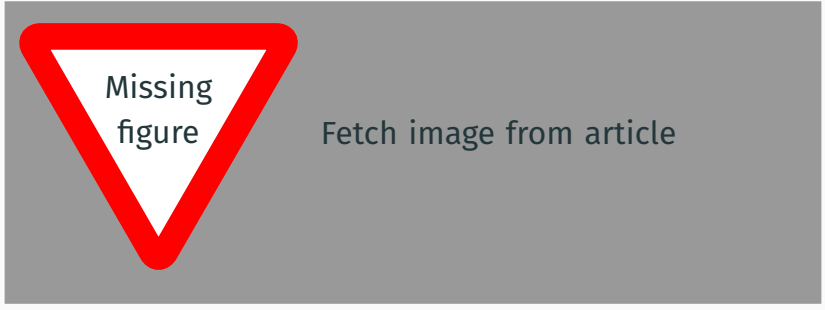
Molecular fingerprinting

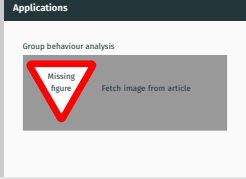




Applications

Group behaviour analysis





GNNs in action

GNNs in action

Thank you

rf.almeida@campus.fct.unl.pt

Thank you
rf.almeida@campus.fct.unl.pt