程序代写代做 CS编程辅导

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Gra omaly Detection

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COMP90073
Security Analytics

Sarah Erfani, CIS

Semester 2, 2021

Outline

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- Why graphs?
- Extracting features from g
- Random walk
- Graph Convolutional Networks (GCNs)

All Real-world Data Does Not "Live" on Grid

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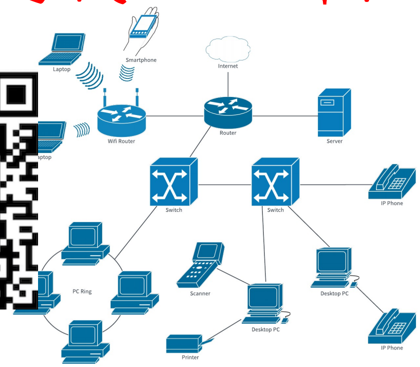
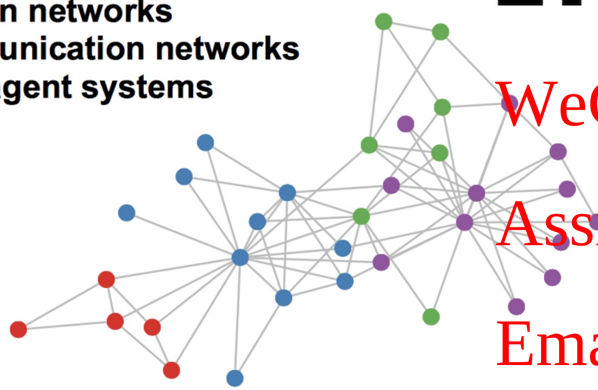
Inte
IoT



Social networks
Citation networks
Communication networks
Multi-agent systems



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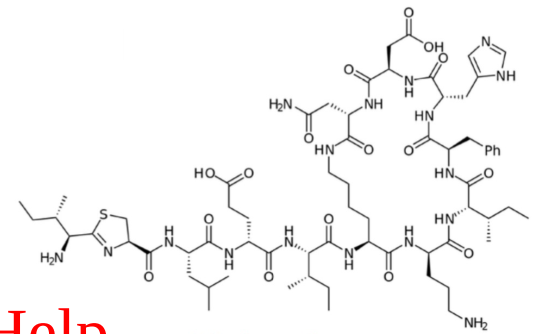
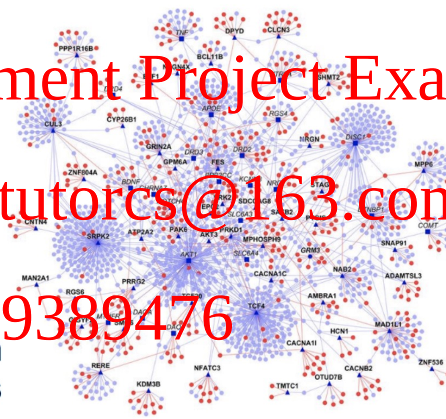


Molecules



Protein interaction networks

Road maps

Outliers vs. Graph Anomalies

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- Anomalies answer the question of *what is interesting about a network*
- Cannot always be treated lying in a multi-dimensional space independently
- They may exhibit inter-de s

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Figure. Graph-based anomaly detection (left) vs. Point-based anomaly detection (right).

Automating Botnet Detection with Graph Neural Networks [3]

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Figure: An example of CAIDA networks embedded with a synthetic P2P botnet. Most of the red botnet nodes are able to reach the rest of the botnet within several hops. The botnet has a faster mixing rate than the background network.

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Why Graphs?

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- **Inter-dependent nature of the data**: Data objects are often related to each other and exhibit depende[illegible]st relational data can be thought of as inter-dependent, which necessi[illegible]ccount for related objects in finding anomalies.

- **Powerful representation:** The multiple paths lying between objects effectively capture their long-range correlations. Moreover, a graph representation facilitates the representation of rich datasets enabling the incorporation of node and edge attributes/types

- **Relational nature of problem domains:** The nature of anomalies could exhibit themselves as relational.

- **Robust machinery:** One could argue that graphs serve as more adversarially robust tools.

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Graph-specific Challenges

- **Inter-dependent Objects:** The relational nature of the data makes it challenging to quantify the [illegible]usness of graph objects. While in traditional anomaly detection, the ob[illegible]ta points are treated as independent and identically distributed (i.i.d[illegible]ch other, the objects in graph data have long-range correlations.

- **Variety of Definitions:** The definitions of anomalies in graphs are much more diverse than in traditional anomaly detection, given the rich representation of graphs.

- **Size of Search Space:** The enumeration of possible substructures is combinatorial which makes the problem of finding out the anomalies a much harder task. This search space is enlarged even more when the graphs are attributed as the possibilities span both the graph structure and the attribute space.

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Machine Learning Lifecycle

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Raw Data → Feature → Learning Algorithm → Model

Features From Graphs

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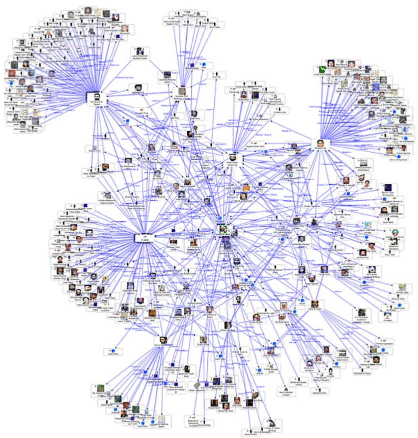
Aim: *Efficient task-independent* feature learning for machine learning with graphs!



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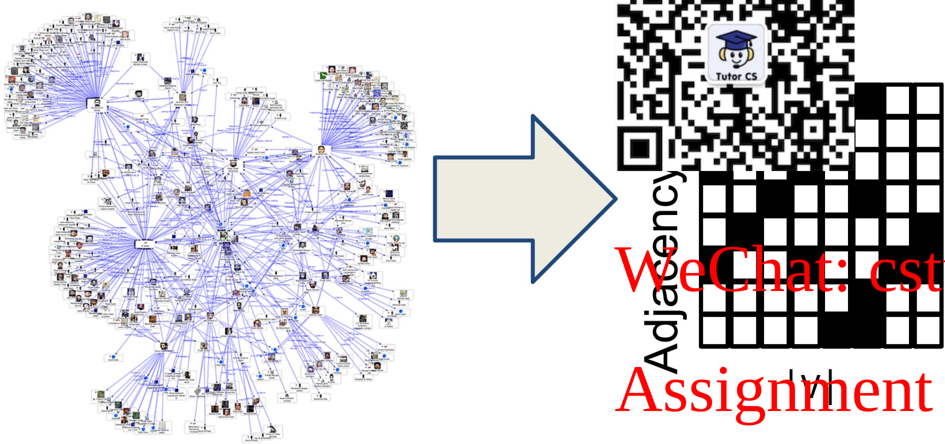

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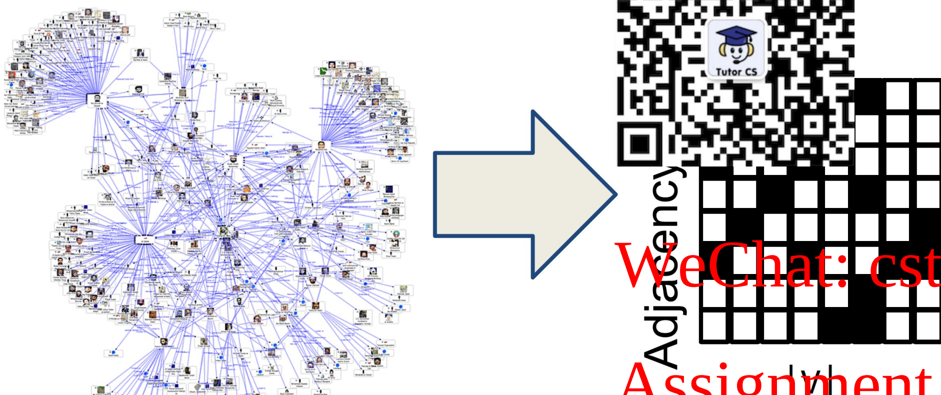

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Basic approaches to extract graph features:

- Adjacency matrix
- node: degree
- pairs: # of common neighbours
- groups: cluster assignments

Features From Graphs

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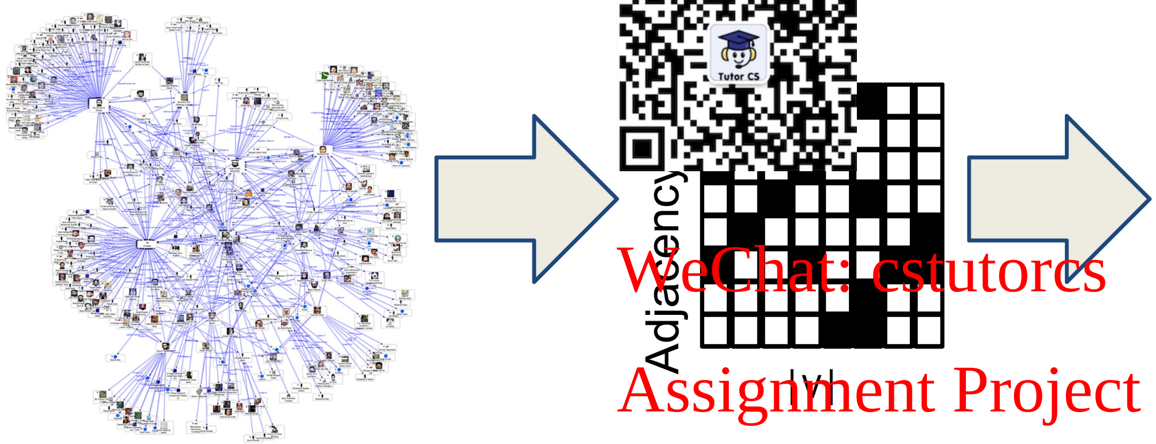
Aim: *Efficient task-independent* feature learning for machine learning with graphs!



- Anomaly Detection
- Attribute Prediction
- Clustering
- Link Prediction
- ...

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Basic approaches to extract graph features:

- Adjacency matrix
- node: degree
- pairs: # of common neighbours
- groups: cluster assignments

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Node Embedding (Representation Learning)

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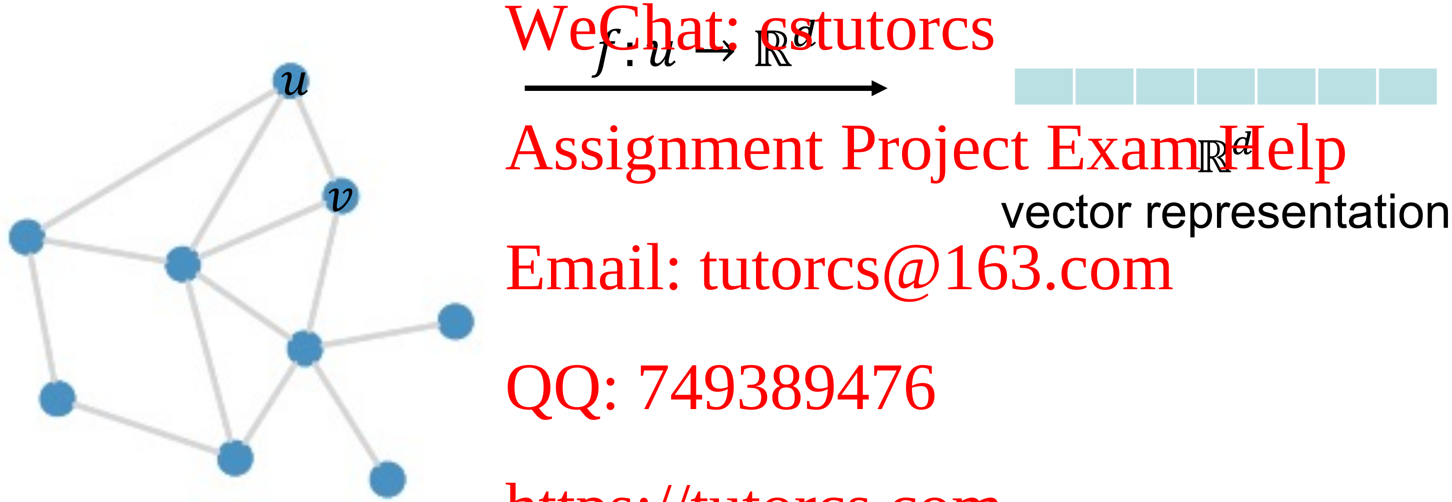
- **Idea:** Map each node in a network into a low-dimensional space



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Why Node Embedding?

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- Encode network information and generate node representation
- Distributed representatio[illegible]es
- Similarity of embeddings [illegible]odes indicates their network similarity

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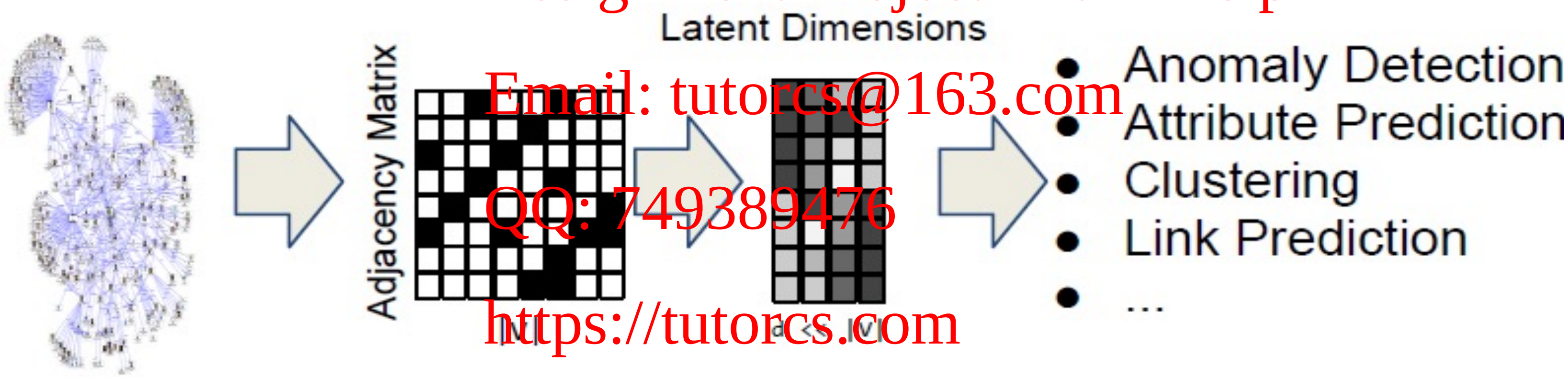

Illustrative Example of Node Embedding

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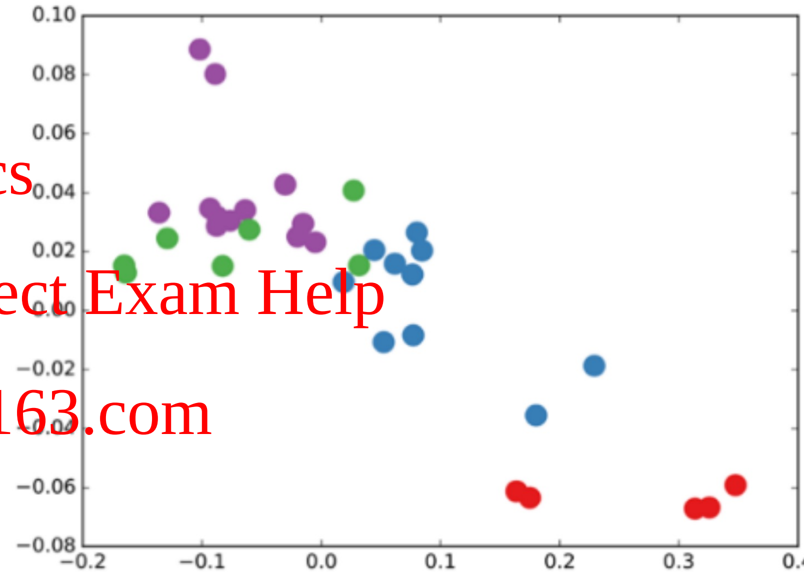
f(

) =



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Input **Output**

Why Node Embedding is Hard?

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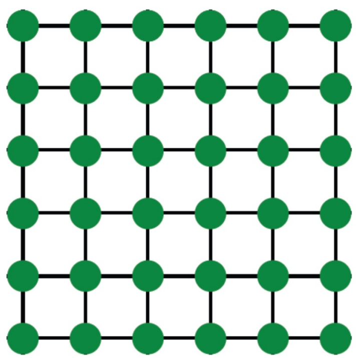
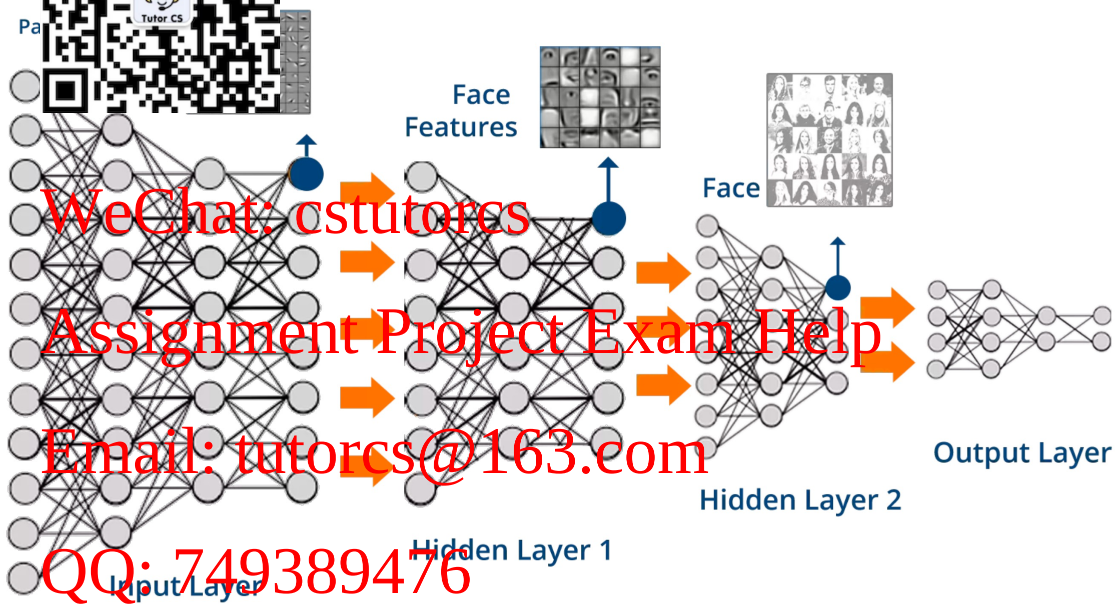
- Modern machine learning toolboxes are designed for data defined on Euclidean domains (with simple sequences and grids).



Images



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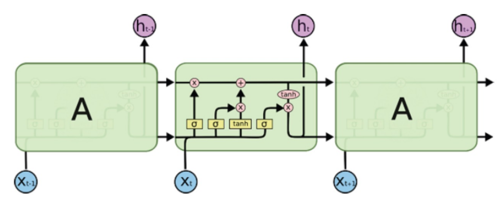
Text/Speech



Why Node Embedding is Hard?

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- But graphs are far more complex!
- Complex topographical st… e., no spatial locality like grids)
- No fixed node ordering or … point (i.e., the isomorphism problem)
- Often dynamic and have multimodal features.

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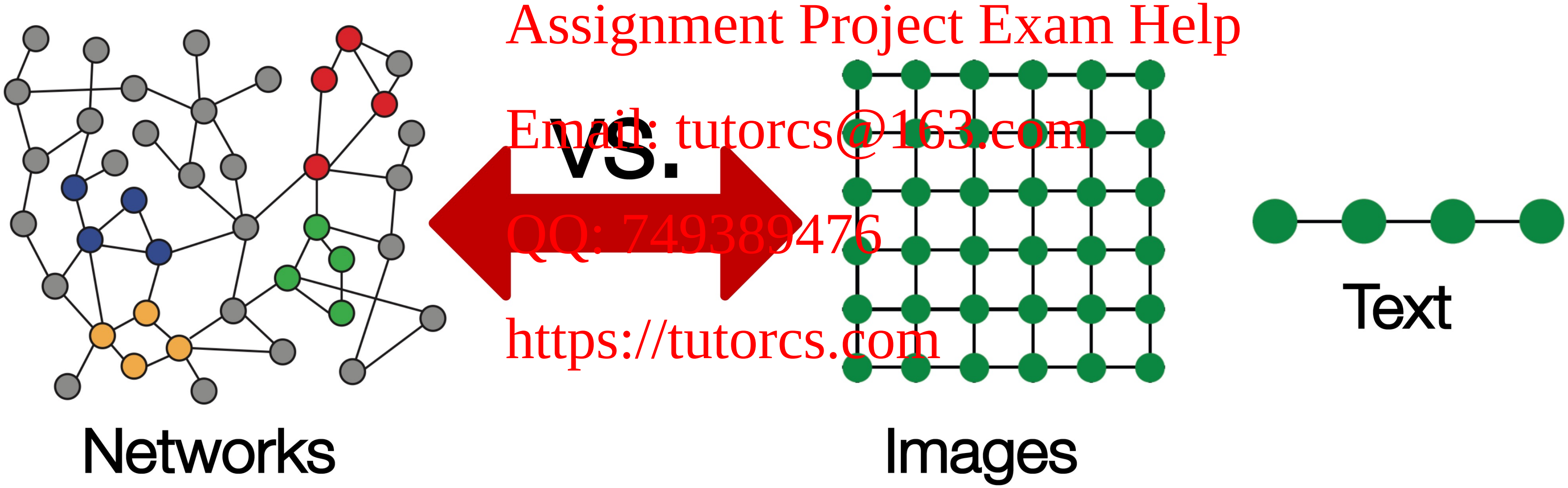

Applications of Graph Embeddings

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- **Node Related Applications:** Node Classification and semi-supervised learning, Anomaly detecti[illegible] Recommendation/Retrieval/Ranking, Clustering and community[illegible].

- **Edge Related Applicatio[illegible]**[illegible]Prediction and Graph Reconstruction.

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- **Graph Related Application:** Graph Classification, Visualization and pattern discovery, Network compression.

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Input Graph   Node Embedding   Edge Embedding   Graph Embedding

Node Embedding

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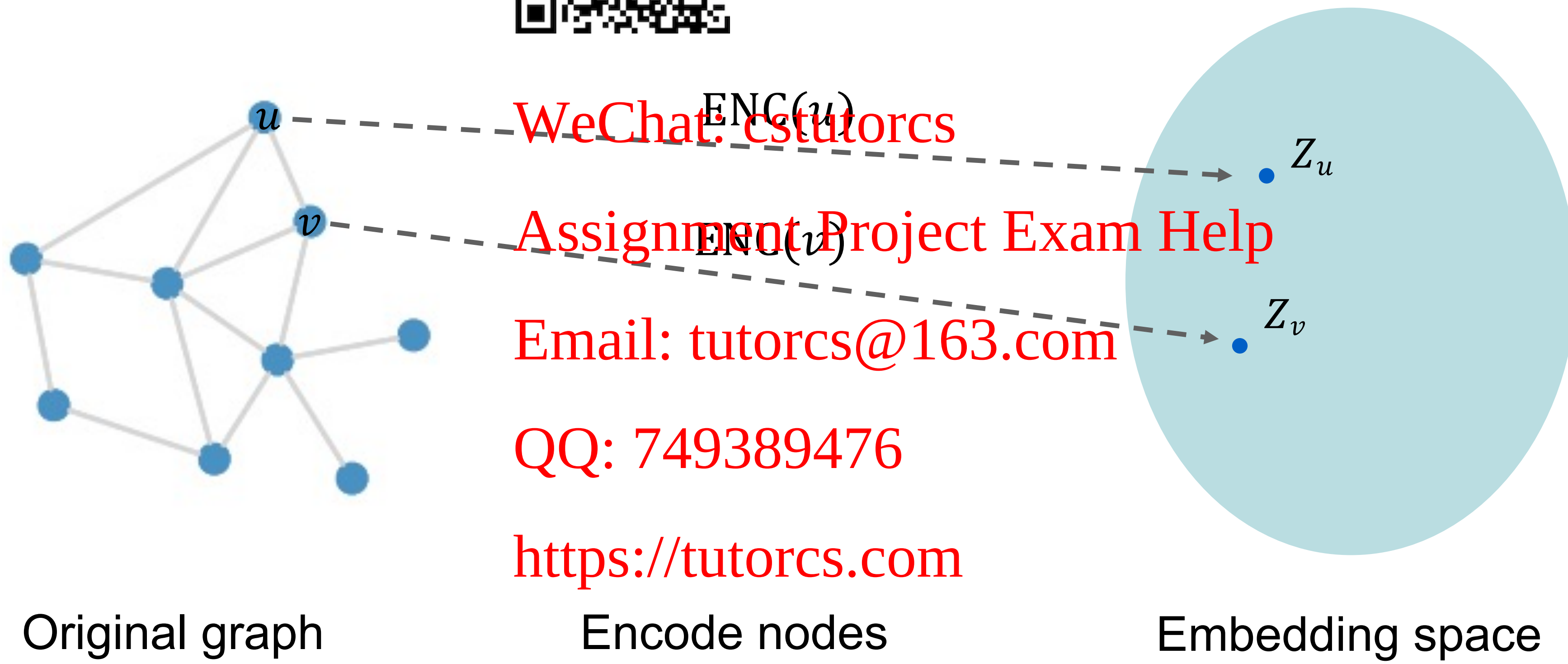
- **Aim:** Encode nodes so that similarity in the embedding space (e.g., dot product) approximates similarity in the original graph



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Node Embedding

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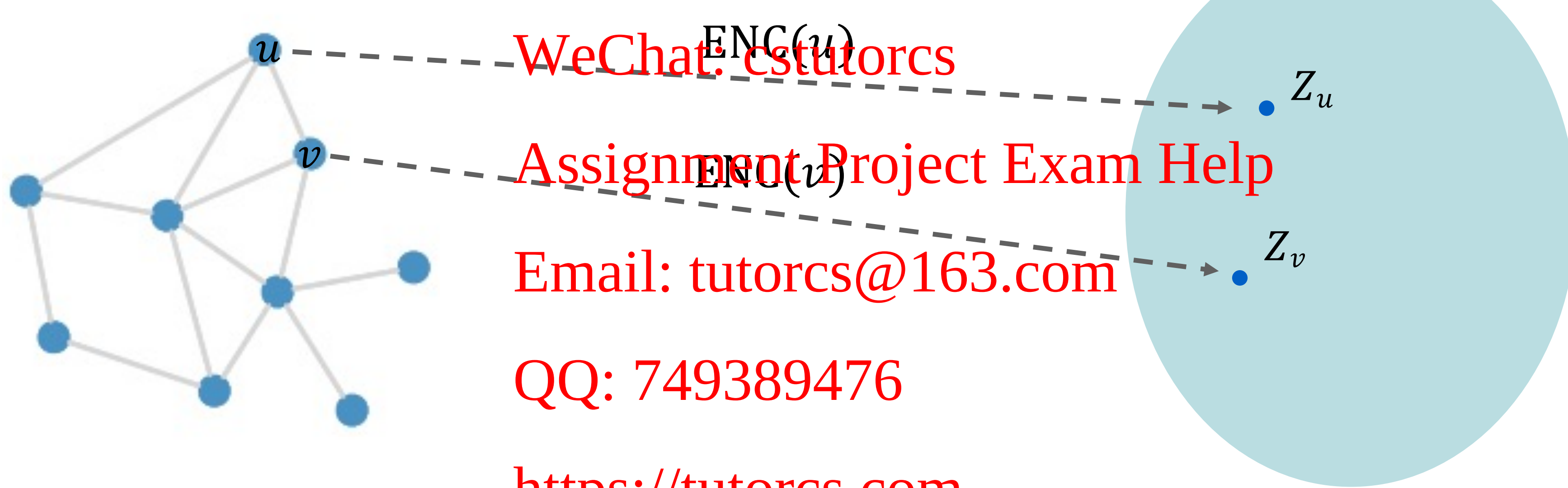
$$similarity(u, v) \approx Z_v \cdot Z_u$$



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Original graph Encode nodes Embedding space

Learning Node Embeddings

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1. Define a node similarity function (i.e., a measure of similarity in the original graph)

   – **Similarity function:** specifies how the relationships in vector space map to the relationships in the original graph

2. Define an encoder (i.e., a mapping from nodes to embeddings)

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   – **Encoder:** maps each node to a lowdimensional vector

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$$\mathrm{ENC}(u) = Z_u \longrightarrow \text{d dimensional}$$

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3. Optimize the parameters of the encoder so that:

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$$similarity(u, v) \approx Z_v \cdot Z_u$$

Random Walk

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Assume we have a graph G:

- V is the vertex set.
- $\boldsymbol{A}$ is the adjacency matrix ...binary).
- *No node features or extra information is used!*

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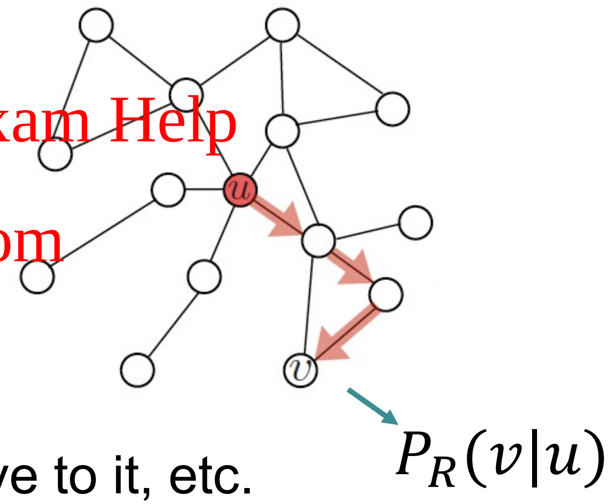
General Idea of Random Walk:



- Given a graph and a starting point,
- Select a neighbour of it at random,
- Move to this neighbour;
- Select a neighbour of this point at random, and move to it, etc.
- Estimate probability of visiting node v on a random walk starting from node u using some random walk strategy R

Random Walk Embedding

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Aim: Build an embedding lookup, where each node is assigned to a unique *d*-dimensional embedding vector that preserves similarity.

- Given $G = (V, E)$
- Run short fixed-length random walks starting from each node u on the graph using some strategy R
- For each node u collect $N_R(u)$, the set of nodes visited on random walks starting from u
- Goal is to learn a mapping $z: u \to \mathbb{R}^d$
- Given node u, we want to learn feature representations that are predictive of the nodes in its neighbourhood $N_R(u)$

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Random Walk Embedding Optimization

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Intuition: Optimize embeddings to maximize likelihood of random walk co-occurrences (using Stochastic Gradient Descent)

$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log(P(v|\mathbf{z}_u)) \longrightarrow$$

Predicted probability of u and v co-occurring on random walk

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- Parameterize $P(v|\mathbf{z}_u)$ using softmax

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$$P(v|\mathbf{z}_u) = \frac{\exp(\mathbf{z}_u \cdot \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u \cdot \mathbf{z}_n)}$$

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Enhancing Random Walk Optimization

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$$\mathcal{L} = \sum_{u \in V} \sum -\log\left(\frac{\exp(\mathbf{z}_u \cdot \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u \cdot \mathbf{z}_n)}\right)$$

- Nested sum over nodes r[illegible] $|V|^2$) complexity!

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Enhancing Random Walk Optimization

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$$\mathcal{L} = \sum_{u \in V} \sum -\log\left(\frac{\exp(\mathbf{z}_u \cdot \mathbf{z}_v)}{\boxed{\sum_{n \in V} \exp(\mathbf{z}_u \cdot \mathbf{z}_n)}}\right)$$

- Nested sum over nodes r[illegible] $|V|^2$) complexity!

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Enhancing Random Walk Optimization

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$$\mathcal{L} = \sum_{u \in V} \sum_{v \in N_R(u)} -\log\left(\frac{\exp(\mathbf{z}_u \cdot \mathbf{z}_v)}{\boxed{\sum_{n \in V} \exp(\mathbf{z}_u \cdot \mathbf{z}_n)}}\right)$$

- Nested sum over nodes requires $O(|V|^2)$ complexity!

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Negative sampling [7]: Instead of normalizing w.r.t. all nodes, just normalize against k random "negative samples" n_i

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$$\log\left(\frac{\exp(\mathbf{z}_u \cdot \mathbf{z}_v)}{\sum_{n \in V} \exp(\mathbf{z}_u \cdot \mathbf{z}_v)}\right) \approx \log(\underbrace{\sigma}_{\text{Sigmoid}}(\mathbf{z}_u \cdot \mathbf{z}_v)) - \sum_{i=1}^{k} \log(\sigma(\mathbf{z}_u \cdot \mathbf{z}_n)), n_i \sim \underbrace{P_V}_{\text{random distribution over all nodes}}$$

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Advantages of Random Walk

- Unsupervised:
  - learns features that c[illegible] graph structure independent of the labels' distribution.
- Expressivity:
  - Flexible stochastic definition of node similarity
- Efficiency:
  - Does not need to consider all node pairs when training (only need to consider pairs that co-occur on random walks)
  - Easy to parallelize. Several random walkers (in different threads, processes, or machines) can simultaneously explore different parts of the same graph.
  - Relying on information obtained from short random walks make it possible to accommodate *small changes* in the graph structure without the need for global re-computation.

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Drawbacks of Random Walk

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- $O(|V|)$ parameters are needed:
  - Every node has its own embedding
  - No sharing of parameters between nodes
- Inherently "transductive":
  - Cannot generate embeddings for nodes that are not seen during training
- Do not incorporate node features:
  - Many graphs have features that we can and should leverage

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Features Graph Embedding

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Assume we have a graph G:

- V is the vertex set.
- $\boldsymbol{A}$ is the adjacency matrix binary).
- $\boldsymbol{X} \in \mathbb{R}^{m \times |V|}$ is a matrix of node features

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Aim: Generate node embeddings $\boldsymbol{Z} \in \mathbb{R}^{n \times f}$ based on local network neighbourhoods

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- Capturing structure
- Borrowing feature information

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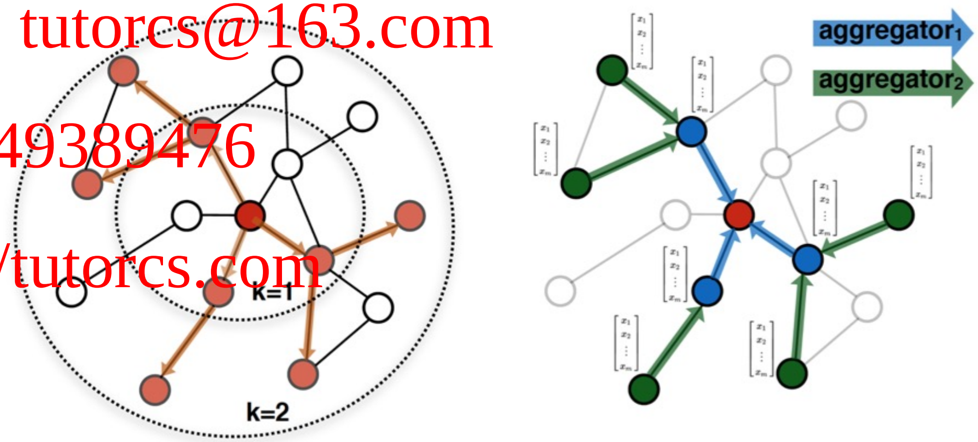
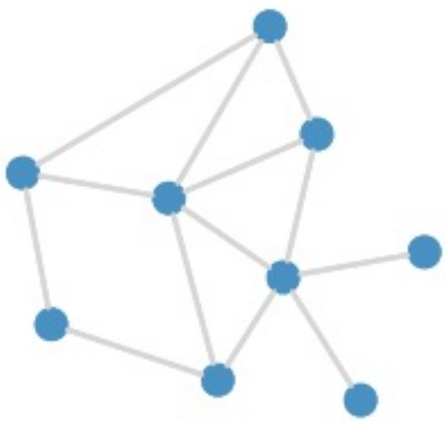


Where Should We Begin?

- Real-world graphs:



or this:

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Naïve Approach

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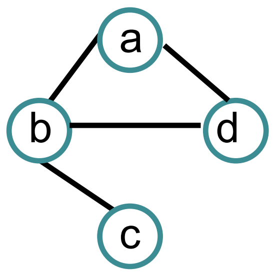
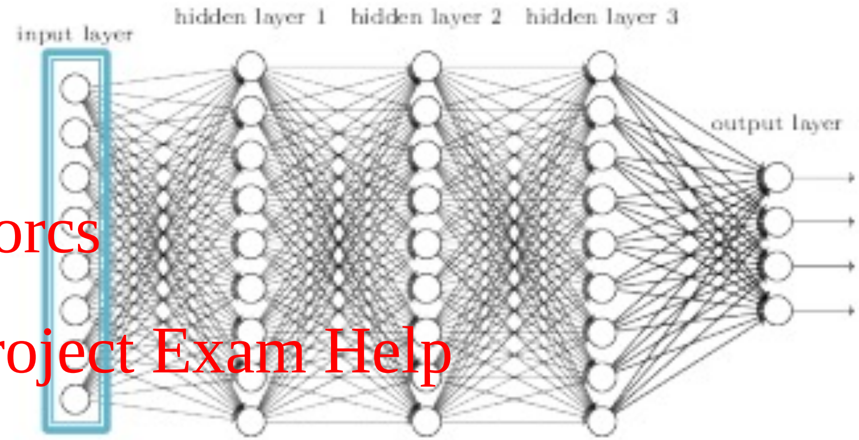
- Join adjacency matrix and features
- Feed them into a deep neural net



$$\begin{array}{c} a \\ b \\ c \\ d \end{array} \begin{pmatrix} \underbrace{\begin{matrix} 0 & 1 & 0 & 1 \\ 1 & 0 & 1 & 1 \\ 0 & 1 & 0 & 0 \\ 1 & 1 & 0 & 0 \end{matrix}}_{A} & \underbrace{\begin{matrix} 0 & 1 \\ 0 & 1 \\ 1 & 1 \\ 0 & 1 \end{matrix}}_{X} \end{pmatrix}$$



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Issues with this approach:

- Large number of parameters
- Not applicable to graphs of different sizes
- Not invariant to node ordering

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Intuition of Graph Convolutional Neural Network (GCN)

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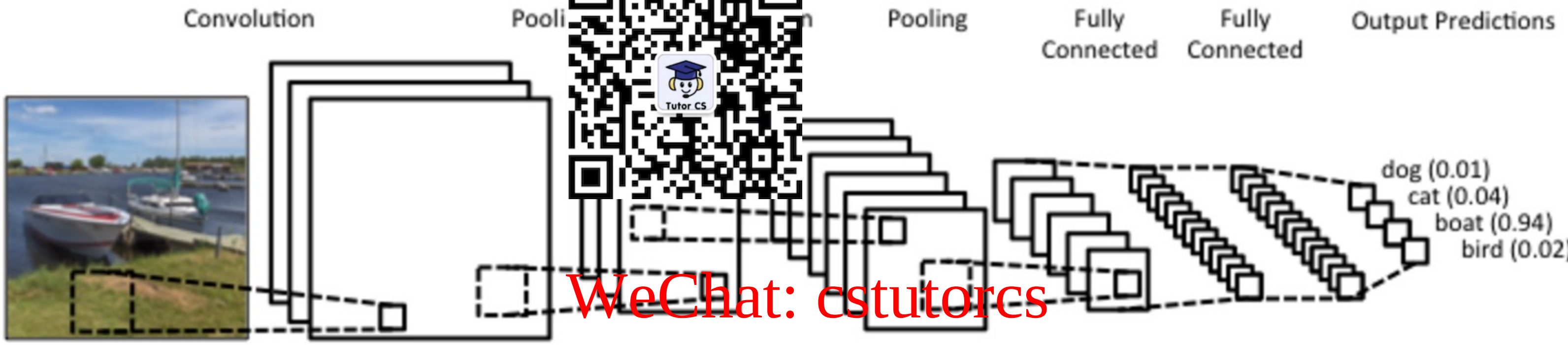
- Revisiting CNN:



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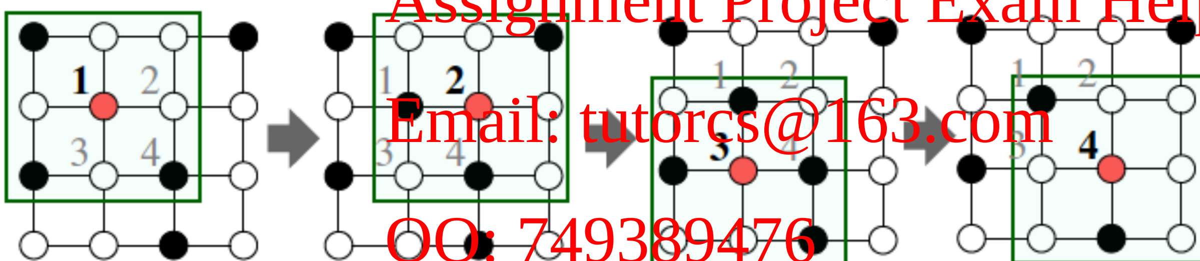

- Goal is to generalize convolutions beyond simple lattices
- Leverage node features/attributes (e.g., text, images)

Intuition of GCN: From Images to Graphs

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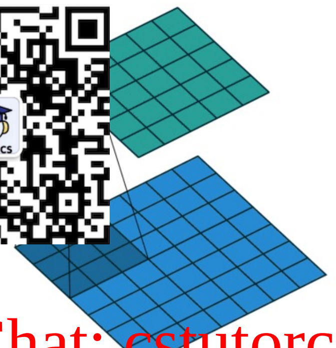
Image: Single CNN layer with 3x3 filter:



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Graph: Transform information at the neighbours and combine it:

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- Transform "messages" h_i from neighbours: $W_i h_i$
- Add them up: $\sum W_i h_i$

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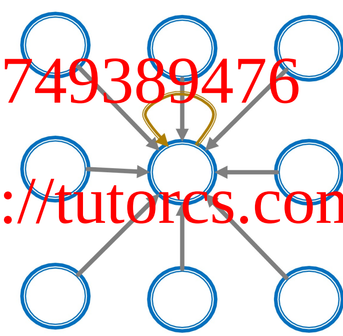

Intuition of GCN: From Images to Graphs [4]

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Figure. 2D Convolution vs. Graph Convolution

Multi-layer Graph Convolutional Network (GCN)

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GCN

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- **Idea:** Node's neighbourhood defines its computation graph
- Learn how to propagate ir across the graph to compute node features

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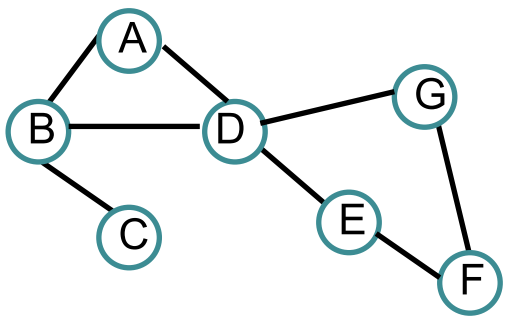

Input graph

GCN

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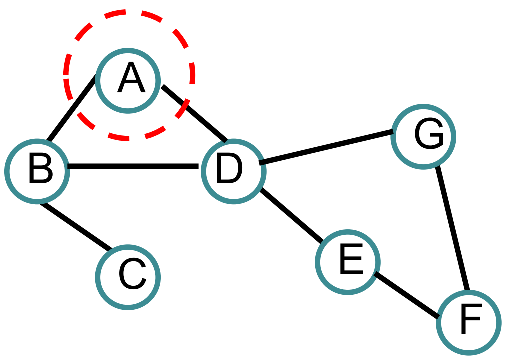
- **Idea:** Node's neighbourhood defines its computation graph
- Learn how to propagate i[illegible] across the graph to compute node features



Input graph

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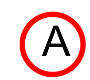

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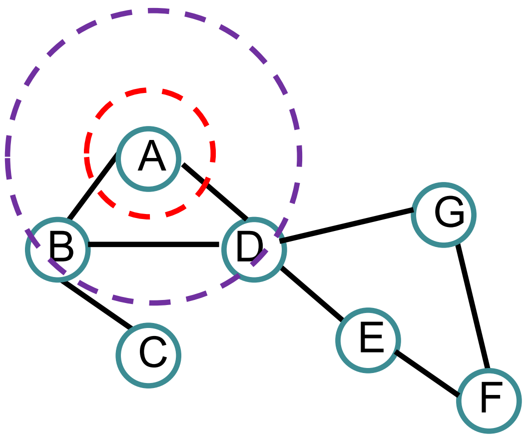

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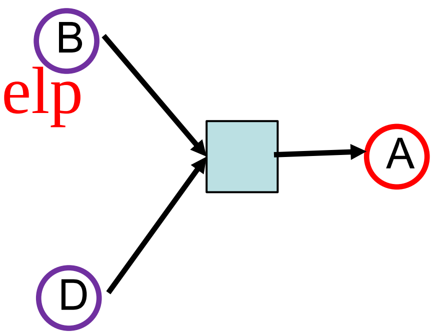

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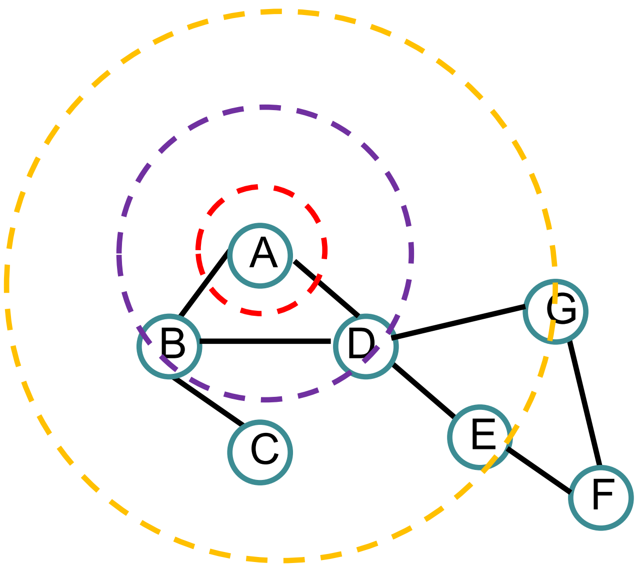

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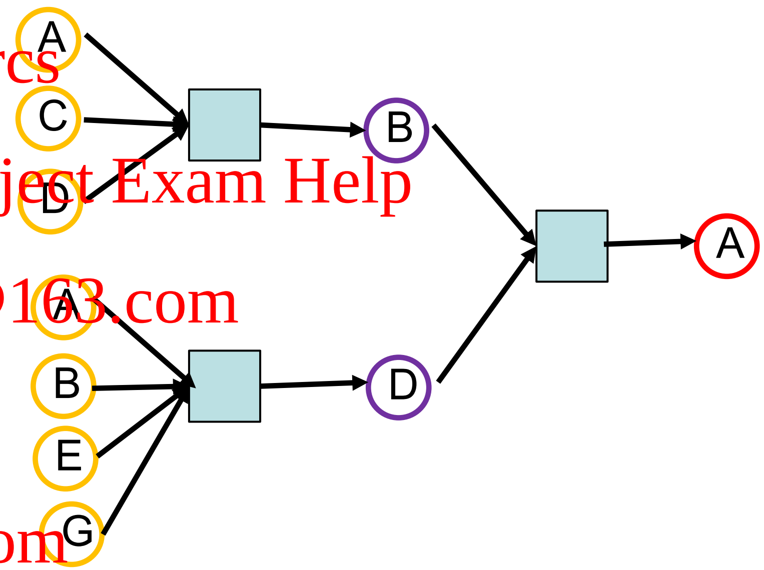

Neighbourhood Aggregation

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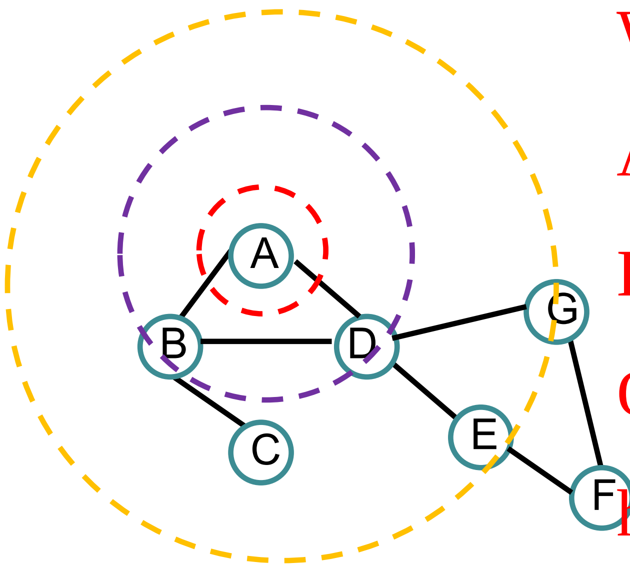
Model can be of arbitrary depth:

- Nodes have embeddings [illegible]yer
- Layer-0 embedding of no[illegible]nput feature, x_u
- Layer-K embedding gets i[illegible] from nodes that are K hops away



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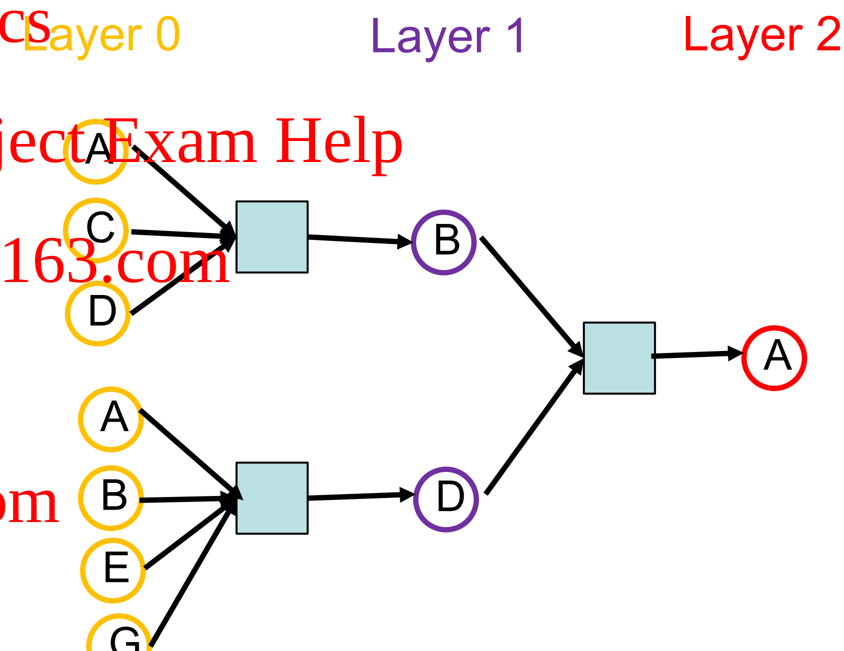

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Information Aggregation

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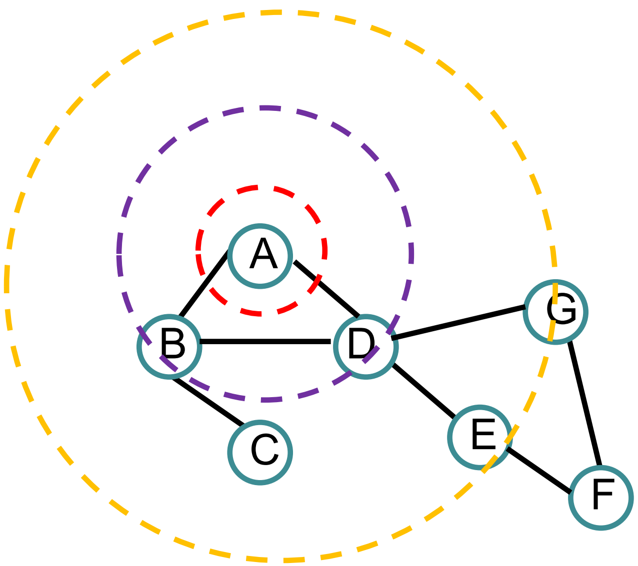
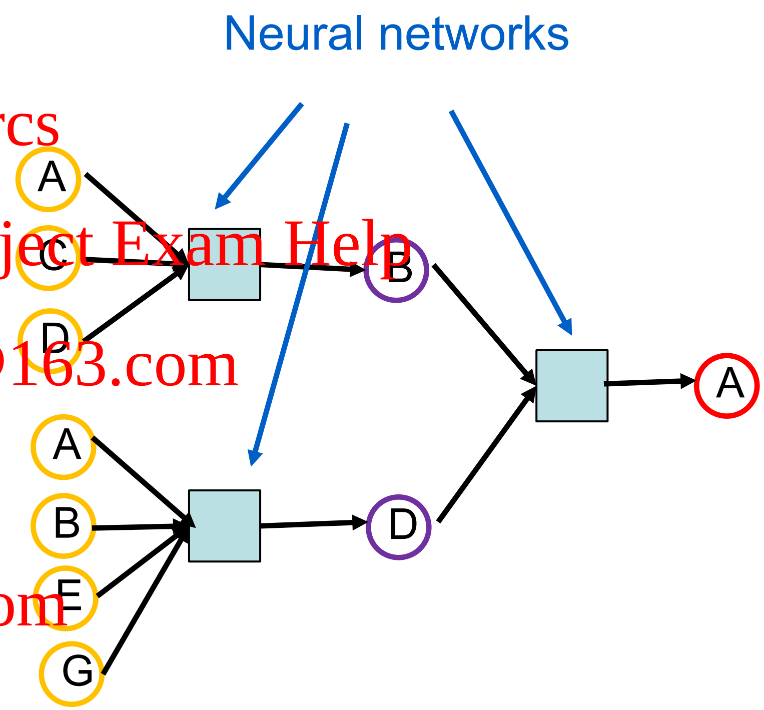
- Intuition: Nodes aggregate information from their neighbours using neural networks
- Every node defines a computation graph based on its neighbourhood!



Input graph



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Neighbourhood Aggregation Functions

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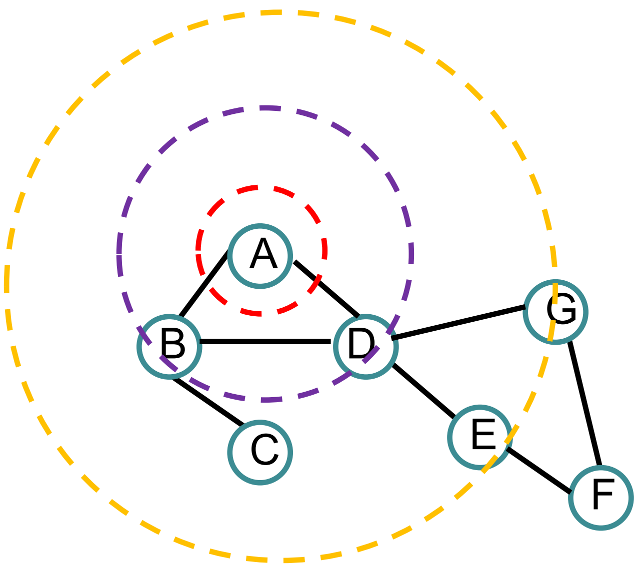
- Neighbourhood aggregation: Key distinctions are in how different approaches aggregate information acr[illegible]yers



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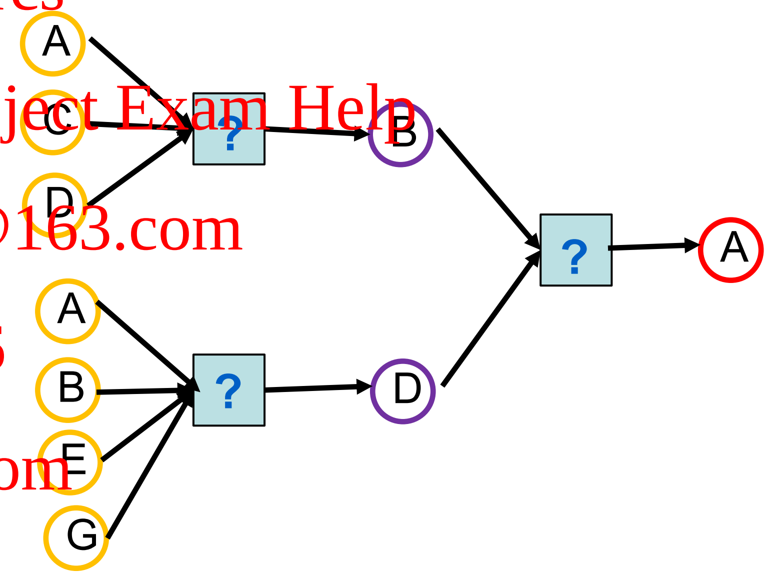

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Neighbourhood Aggregation Functions

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- Basic approach: Average information from neighbour and apply a neural network

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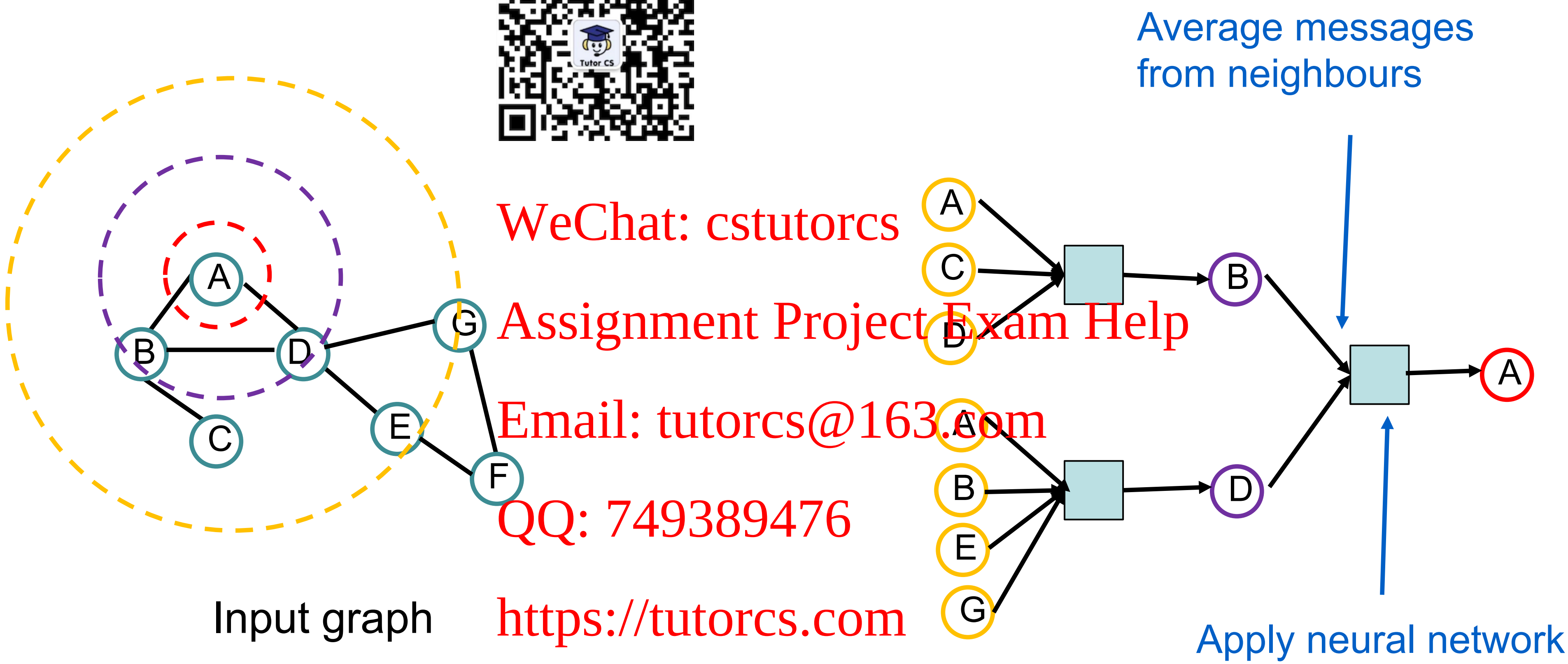

Input graph

Deep Encoder Formulation

程序代写代做 CS编程辅导

- Basic approach: Average neighbour messages and apply a neural network

$$h_v^0 = x_v$$

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$$h_v^k = \sigma\left(W_k \sum_{u \in N(v)} \frac{h_u^{k-1}}{|N(v)|} + B_k h_v^{k-1} \right), \forall k \in \{1, \dots, K\}$$

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$$z_v = h_v^K$$

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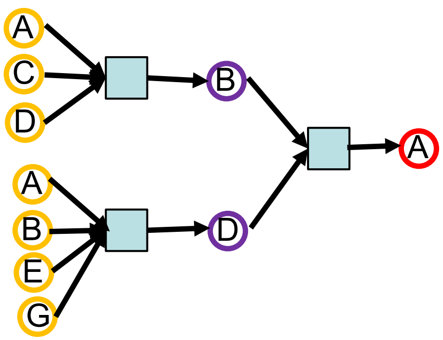

Deep Encoder Formulation

程序代写代做 CS编程辅导

- Basic approach: Average neighbour messages and apply a neural network

$$\mathrm{h}_v^0 = \mathrm{x}_v$$

In[illegible]er
er[illegible]are equal to
node features

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$$\mathrm{h}_v^k = \sigma\left(\mathrm{W}_k \sum_{u \in N(v)} \frac{\mathrm{h}_u^{k-1}}{|N(v)|} + \mathrm{B}_k \mathrm{h}_v^{k-1}\right), \forall k \in \{1, \dots, K\}$$

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$$\mathrm{z}_v = \mathrm{h}_v^{\mathrm{K}}$$

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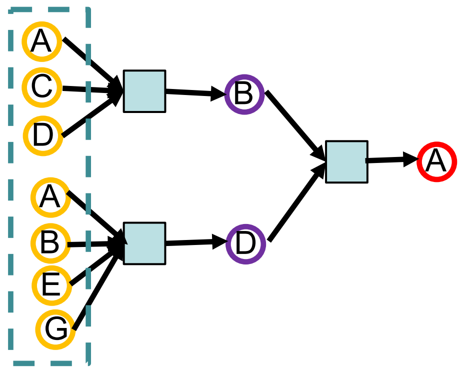

Deep Encoder Formulation

程序代写代做 CS编程辅导

- Basic approach: Average neighbour messages and apply a neural network

$$h_v^0 = x_v$$

In … er
er … are equal to
node features

Previous layer h0 embedding of v

$$h_v^k = \sigma\left(W_k \sum_{u \in N(v)} \frac{h_u^{k-1}}{|N(v)|} + B_k h_v^{k-1}\right), \forall k \in \{1, \ldots, K\}$$

$$z_v = h_v^K$$

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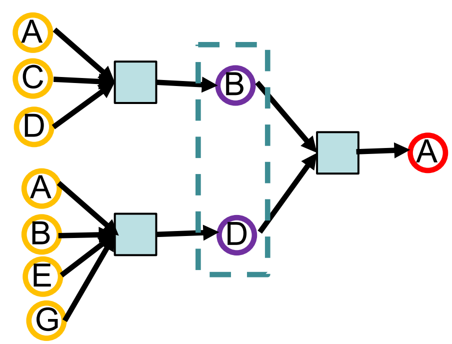

Deep Encoder Formulation

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- Basic approach: Average neighbour messages and apply a neural network

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$$z_v = h_v^K$$

Average of neighbour's
previous layer
embeddings

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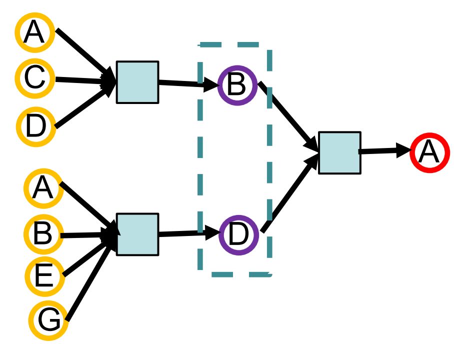

Deep Encoder Formulation

程序代写代做 CS编程辅导

- Basic approach: Average neighbour messages and apply a neural network

In[illegible]er
er[illegible]are equal to
node features

$$h_v^0 = x_v$$

Previous layer h0 embedding of v

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$$h_v^k = \sigma\left(W_k \sum_{u \in N(v)} \frac{h_u^{k-1}}{|N(v)|} + B_k h_v^{k-1}\right), \forall k \in \{1, \dots, K\}$$

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$$z_v = h_v^K$$

Average of neighbour's
previous layer
embeddings

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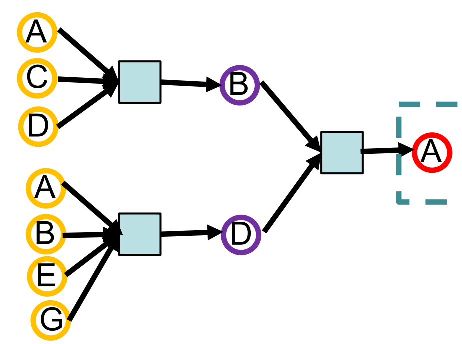
Embedding after K
layers of neighbourhood
aggregation



Training Model Parameters

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- We can feed these embeddings into any loss function and run stochastic gradient descent to train the weight parameters

$$\mathrm{h}_v^k = \sigma\left(\mathrm{W}_k \sum_{u \in N(v)} \frac{\mathrm{h}_u^{k-1}}{|N(v)|} + \mathrm{B}_k \mathrm{h}_v^{k-1} \right)$$

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Trainable parameters

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- Many aggregations can be performed efficiently by (sparse) matrix operations. Let $H^{k-1} = [h_1^{k-1} \ldots h_n^{k-1}]$
  - Mean rule: $H^k = D^{-1} A H^{k-1}$
  - Spectral rule: $H^k = D^{-1/2} A D^{1/2} H^{k-1}$

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Inductive Capability

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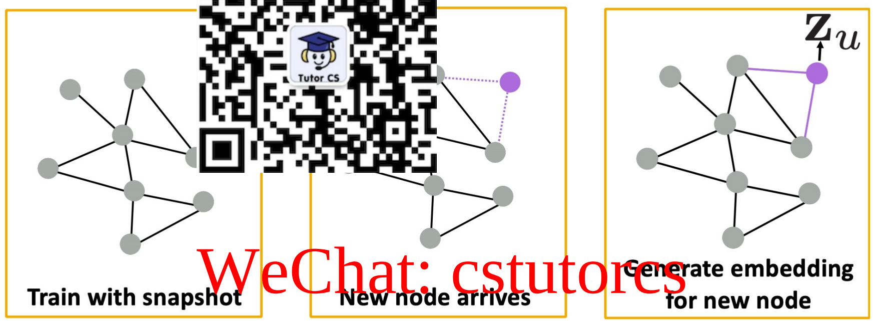
- Many application settings constantly encounter previously unseen nodes



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- Inductive node embedding Generalize to entirely unseen graphs

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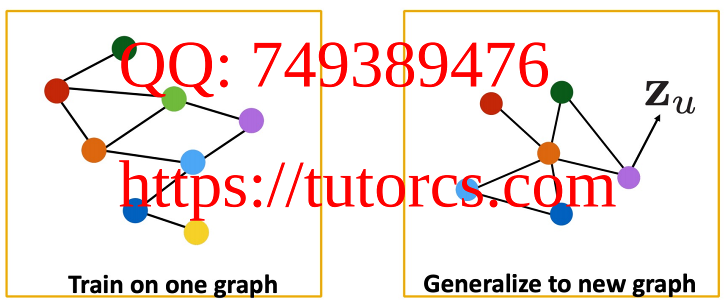

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Variational Graph Autoencoder (VGAE) [4]

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Deep Anomaly Detection on Attributed Networks [7]

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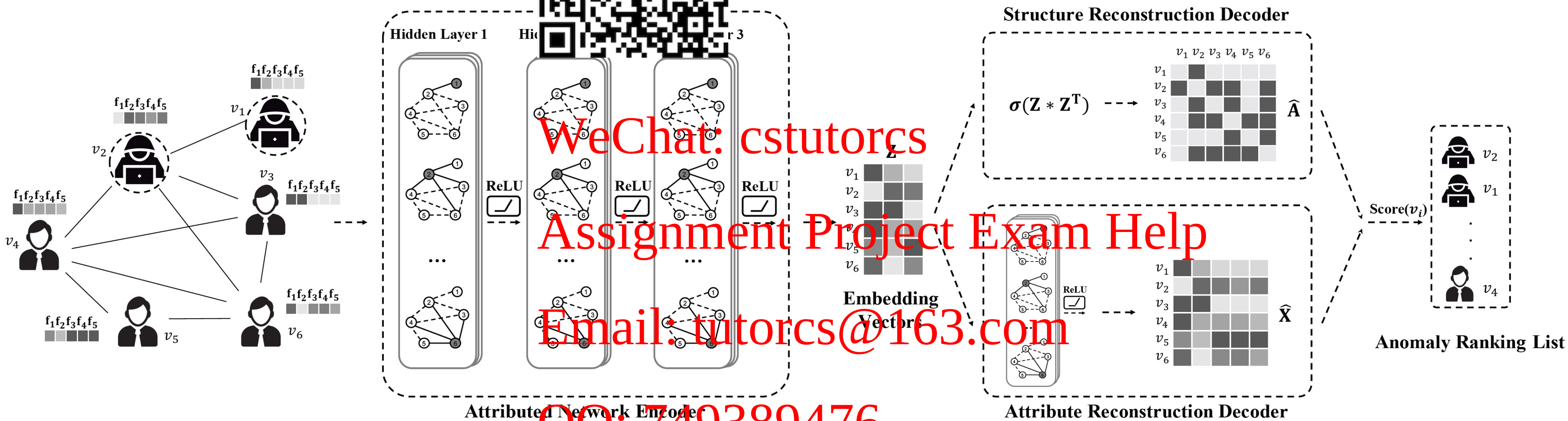

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One-Class Graph Neural Networks for Anomaly Detection in Attributed Networks [5]

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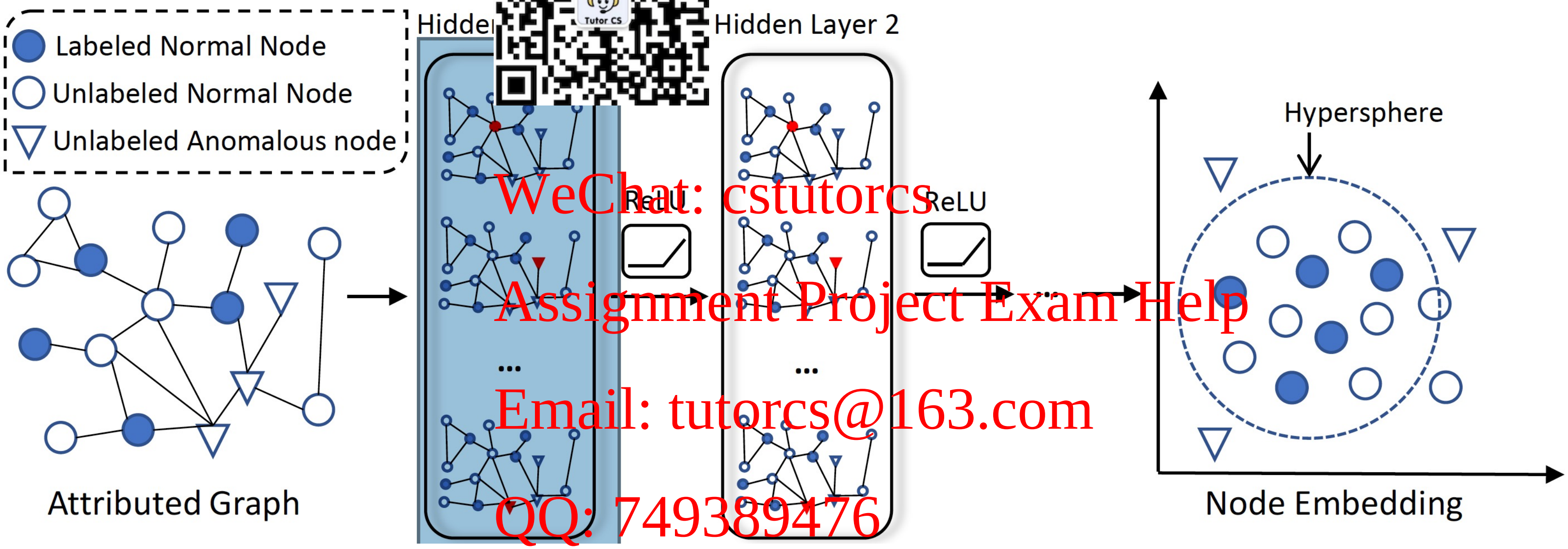

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Summary

程序代写代做 CS编程辅导

- Why it is important to maintain data graph structure?
- How to use random walk f[illegible]ting graph embedding?
- How embed evolving featured graphs?
- How use graph embedding for anomaly detection?

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Next: Contrast Data Mining

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5. Xuhong Wang, Baihong Jin, Ying Du, Ping Cui, and Yupu Yang, "One-Class Graph Neural Networks for Anomaly Detection in Attributed Networks", *arXiv preprint arXiv:2002.09594v2* (2020)

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7. Hongyun Cai, Vincent W[illegible]nd Kevin Chen-Chuan Chang. "A comprehensive survey o[illegible]nbedding: Problems, techniques, and applications." *IEEE Transactions on Knowledge and Data Engineering* 30, no. 9 (2018): 1616-1637.

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