Machine Learning on Graphs

PyTorch London Meetup

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Danish Business Authority

November 3, 2020

An overview of the talk

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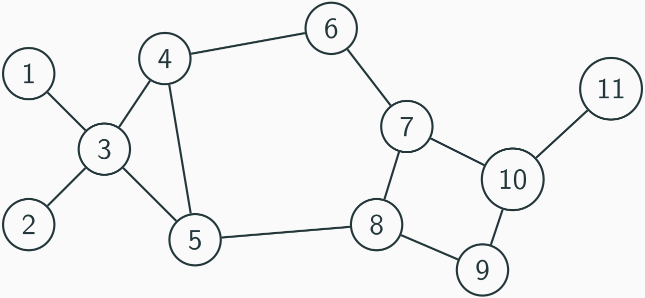
1. What is a graph?
2. Which machine learning tasks can we do on graphs?
   2.1 Node classification
   2.2 Graph classification
   2.3 Link prediction
3. A zoo of algorithms
   3.1 Transductive classification: DeepWalk
   3.2 Inductive classification: Graph convolutions
4. PyTorch implementation
5. Application: Fraud detection

What is a graph?



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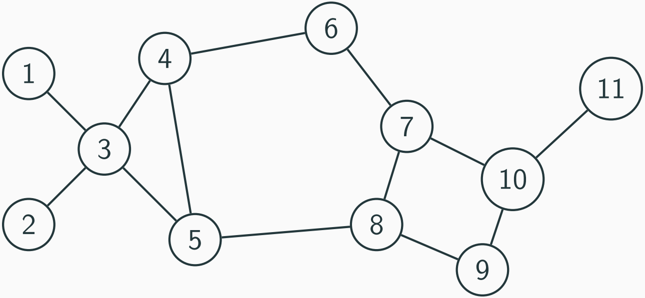
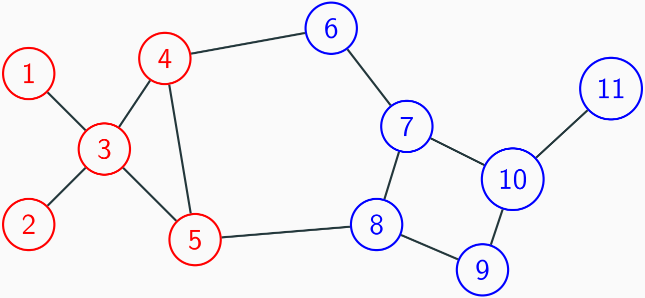
Node classification



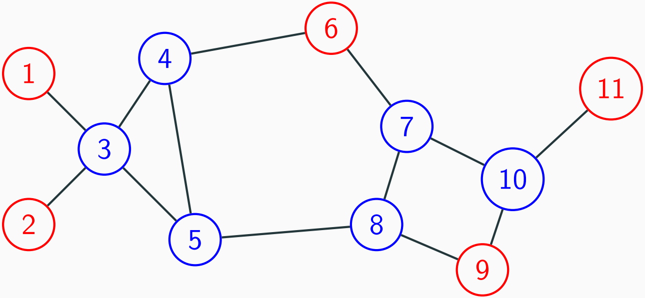
Node classification

Proximity classification:



Node classification

Structural classification:



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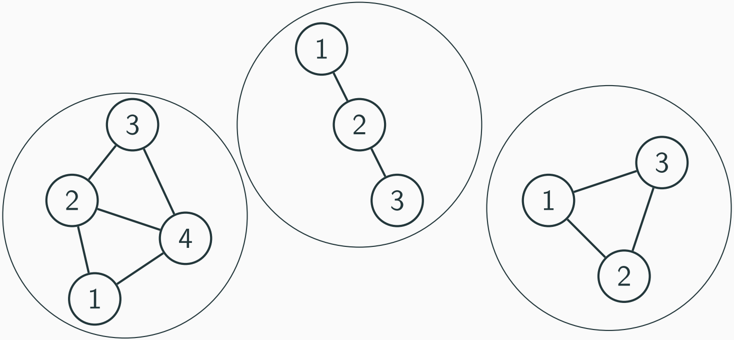

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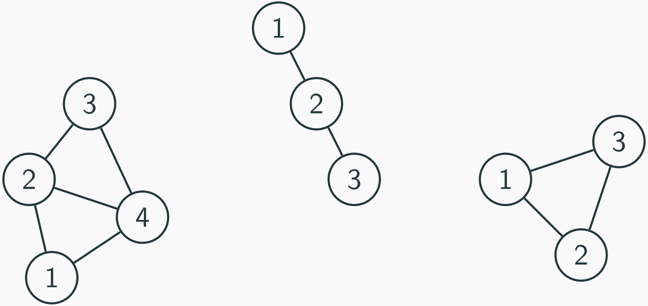

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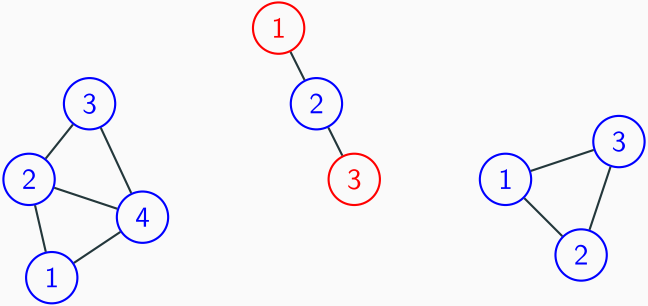

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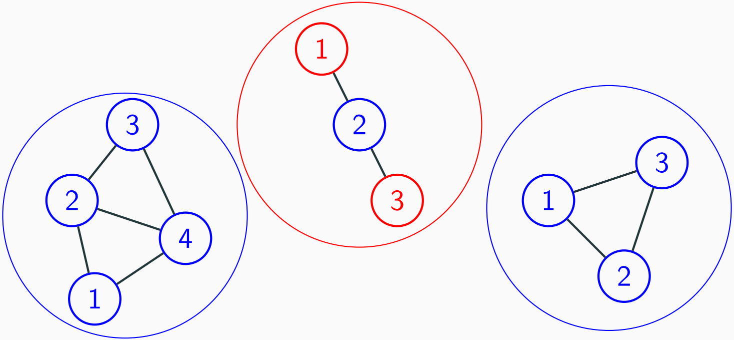

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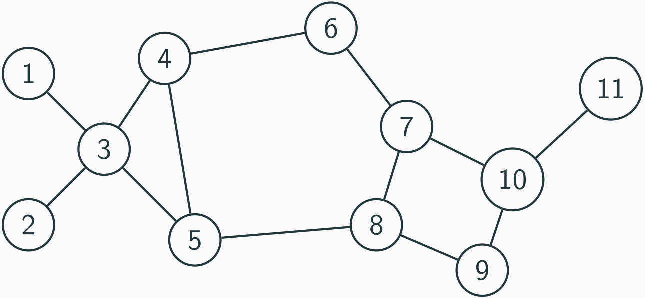
Link prediction



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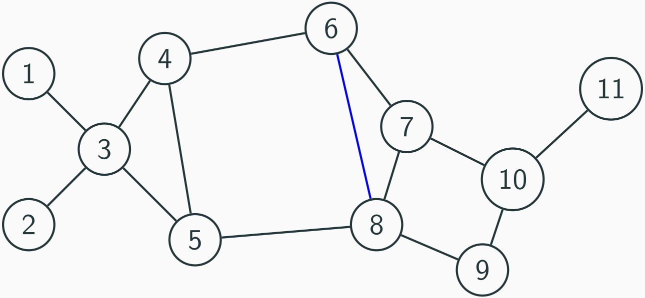

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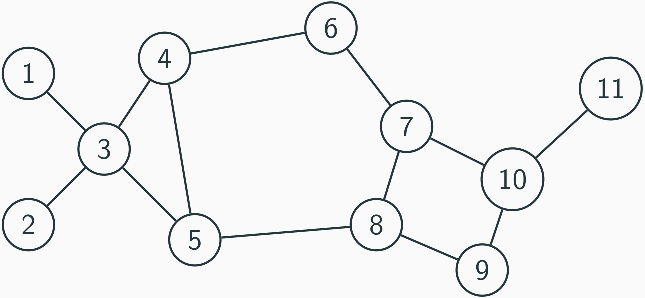
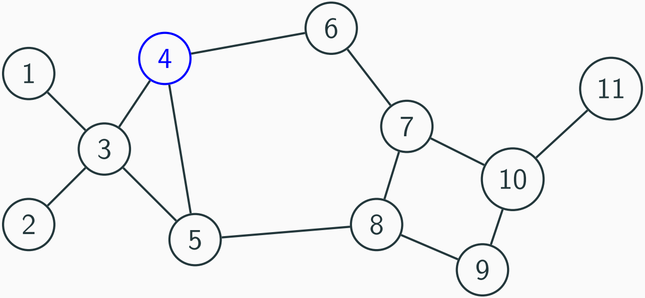


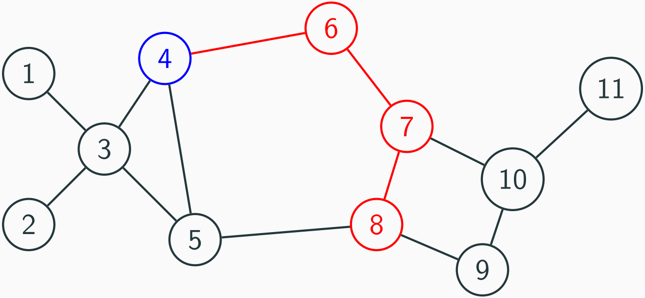
Transductive classification: DeepWalk

For every node...



Transductive classification: DeepWalk

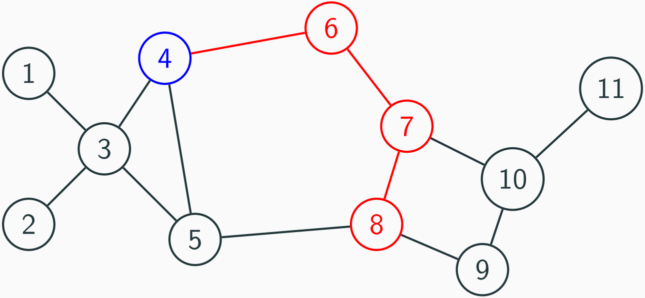
Go for a random walk...



Transductive classification: DeepWalk

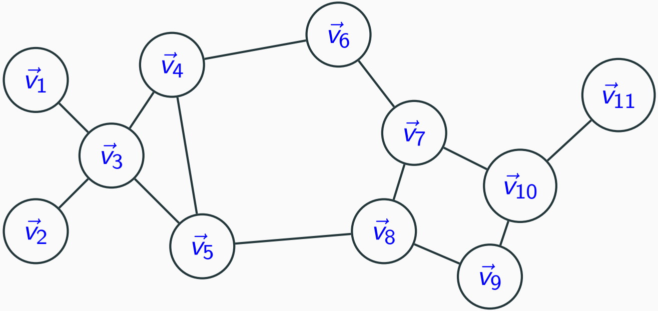
And teach a model to predict the node's neighbours:

$$\texttt{model}(4) \in \{6, 7, 8\}$$



Transductive classification: DeepWalk

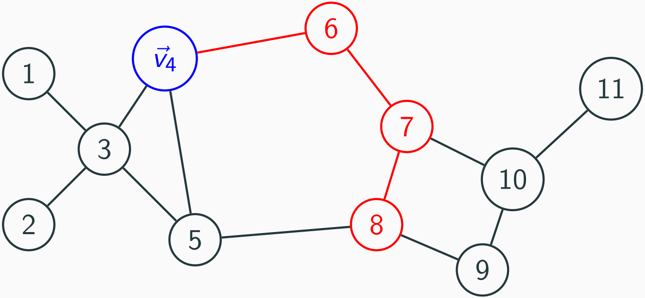
This is done by assigning a learnable vector $\vec{v}_i \in \mathbb{R}^d$ to every node i



Transductive classification: DeepWalk

And training a neural network to predict node indices on the random walk:

$$\mathtt{net}(\vec{v}_4) = (0, 0, 0, 0, 0, \tfrac{1}{3}, \tfrac{1}{3}, \tfrac{1}{3}, 0, 0, 0)$$

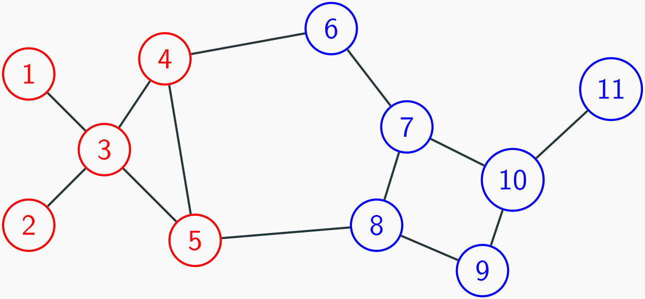


Transductive classification: DeepWalk

From these embeddings we can then train any classification model (say, logistic regression) to get our node labels:

$$\texttt{classificationModel}(\vec{v}_4) \sim 0$$

$$\texttt{classificationModel}(\vec{v}_7) \sim 1$$



Transductive classification: DeepWalk

This algorithm is transductive, meaning that we learn a static embedding (and thus, classification) for every node.

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If a new node appears, we thus have to train all the embeddings from scratch.

Note also that this is, by construction, a proximity classification: nearby nodes will get classified similarly.

An overview of the talk

Inductive classification: Graph convolutions

Let's start with a quick recap of what convolutional neural networks are doing.

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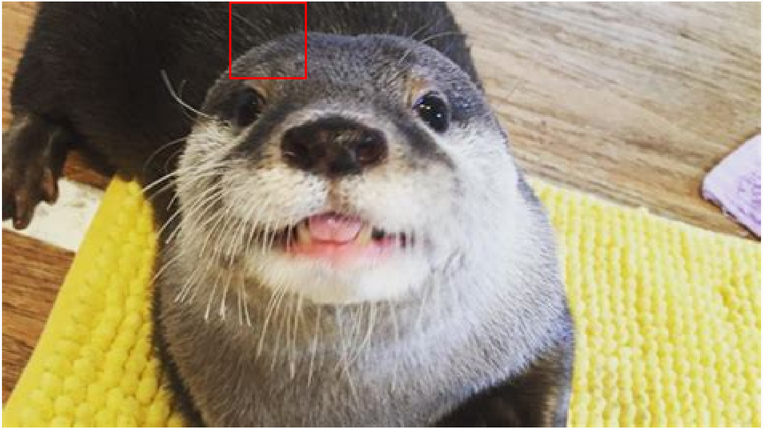

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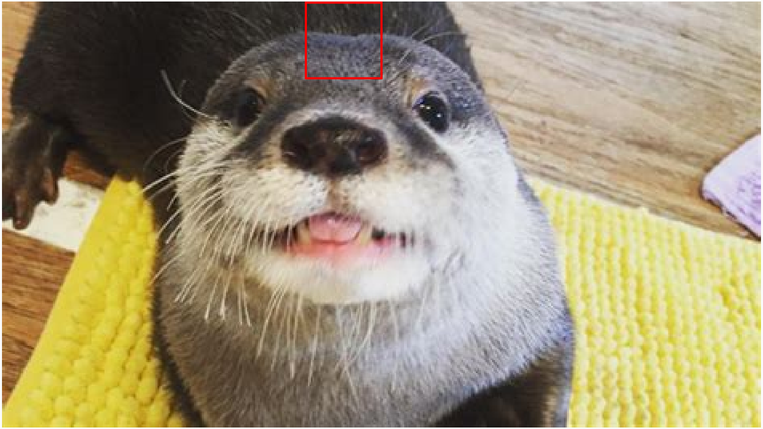

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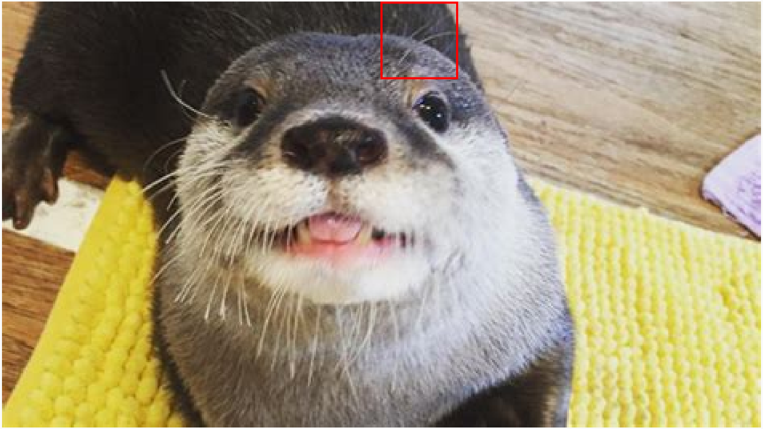

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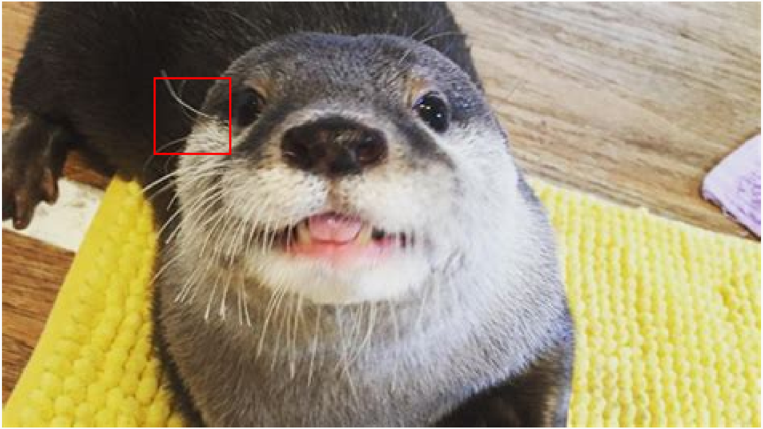

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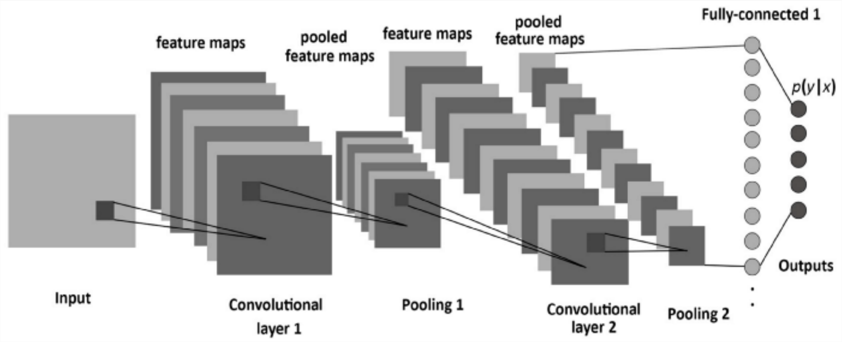

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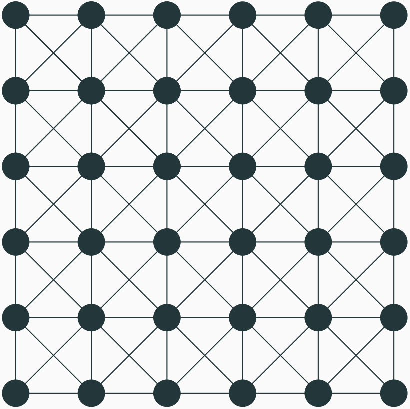
Inductive classification: Graph convolutions

Let's view the cute otter with our graph hat on.

Inductive classification: Graph convolutions



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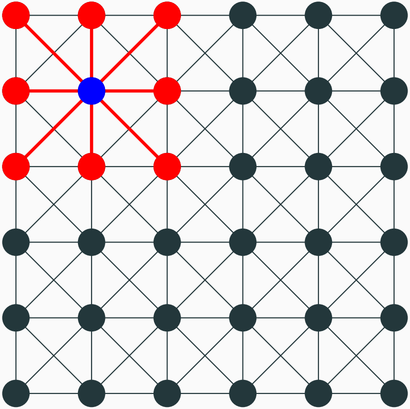

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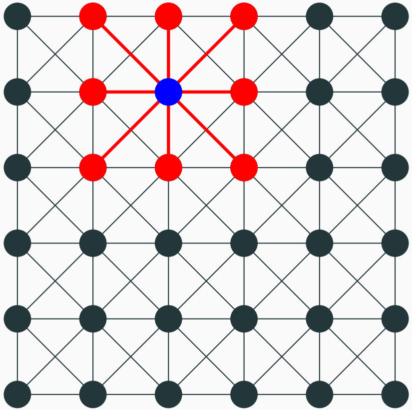

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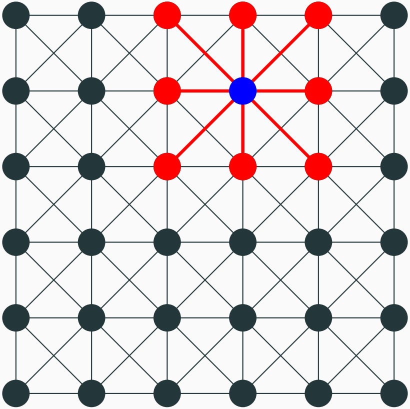

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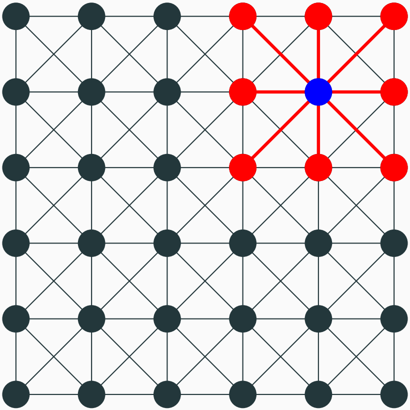

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This makes it possible to learn a 3×3 matrix (the kernel), which we can convolve over:

$$(\texttt{pixels} \star \texttt{kernel})_{m,n} := \sum_{i=-1}^{1} \sum_{j=-1}^{1} \texttt{kernel}_{i,j} \texttt{pixels}_{m-i,n-j}$$

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We lose this feature for general graphs, so what do we do?

Inductive classification: Graph convolutions

MATHS

Inductive classification: Graph convolutions

The Convolution Theorem
Convolutions between two functions $f, g\colon \mathbb{R}^n \to \mathbb{R}$ are equivalent to element-wise multiplication in the Fourier domain:

$$\texttt{fourier}(f \star g) = \texttt{fourier}(f) \cdot \texttt{fourier}(g)$$

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One can define a version of the Fourier transform applied to functions on nodes of a graph, call it `graphFourier`, and then define the graph convolution as

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$$f \star g := \mathtt{graphFourier}^{-1}(\mathtt{graphFourier}(f) \cdot \mathtt{graphFourier}(g))$$

This is called a spectral graph convolution.

Inductive classification: Graph convolutions

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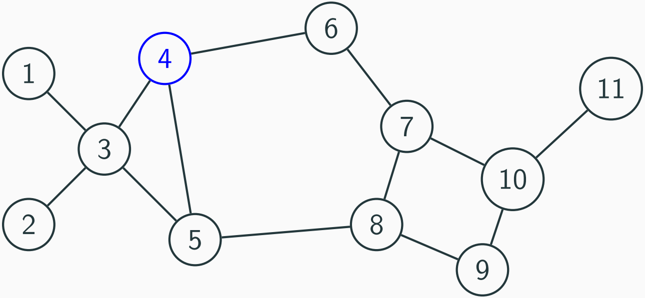
This approximation is also quite simple. Let's have a look.

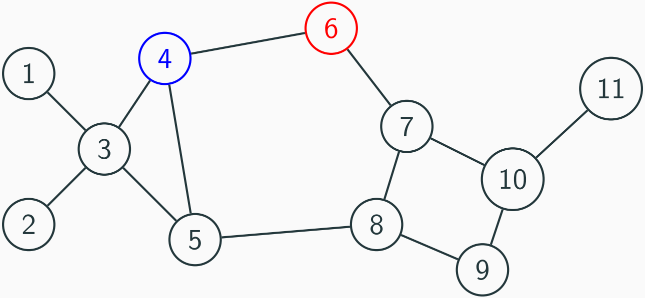
Inductive classification: Graph convolutions

Say we want to compute the convolution at node 4.



Inductive classification: Graph convolutions

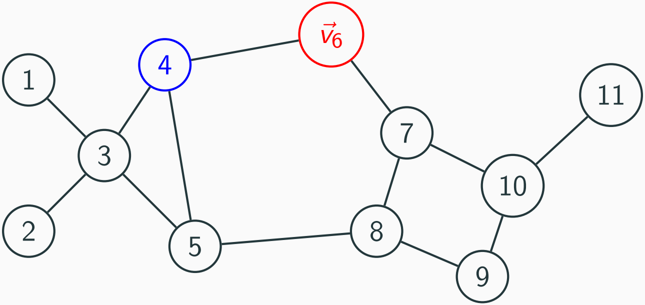
For every neighbour of 4...



Inductive classification: Graph convolutions

We take its feature vector and normalise it by both it's and 4's degrees...

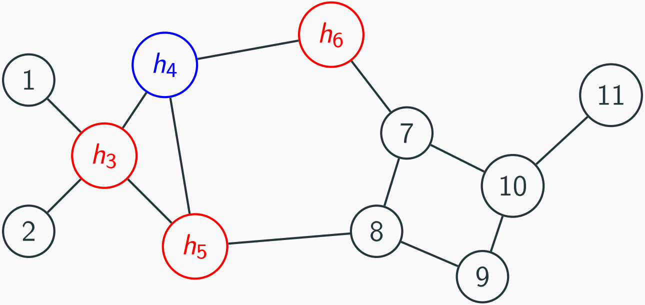
$$h_6 := \frac{\vec{v}_6}{\sqrt{\texttt{degree}(4)\texttt{degree}(6)}} = \frac{\vec{v}_6}{\sqrt{3 \cdot 2}}$$



Inductive classification: Graph convolutions

Node 4's new value is then the sum of the h_i's, multiplied with a learnable weight matrix W:

$$\vec{v}_4 := W(h_4 + h_3 + h_5 + h_6)$$



Inductive classification: Graph convolutions

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As opposed to DeepWalk, the GCNs are inherently supervised, but methods exist to train this in an unsupervised way (e.g. the Deep Graph Infomax algorithm from Veličković et al., 2018)

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PyTorch implementation

Deep Graph Library: `https://www.dgl.ai`

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import torch
import torch.nn as nn
import dgl
import dgl.nn.pytorch as dglnn

class GCN(nn.Module):
    def __init__(self, in_feats:int, hidden_size:int, num_classes:int):
        super().__init__()
        self.conv1 = dglnn.GraphConv(in_feats, hidden_size)
        self.conv2 = dglnn.GraphConv(hidden_size, num_classes)

    def forward(self, graph:dgl.DGLGraph, x:torch.tensor):
        x = self.conv1(graph, x)
        x = torch.relu(x)
        x = self.conv2(graph, x)
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    def forward(self, data:tg.data.Data):
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All companies in Denmark have to register with the authority before they are officially recognised as a company.

Application: Fraud detection

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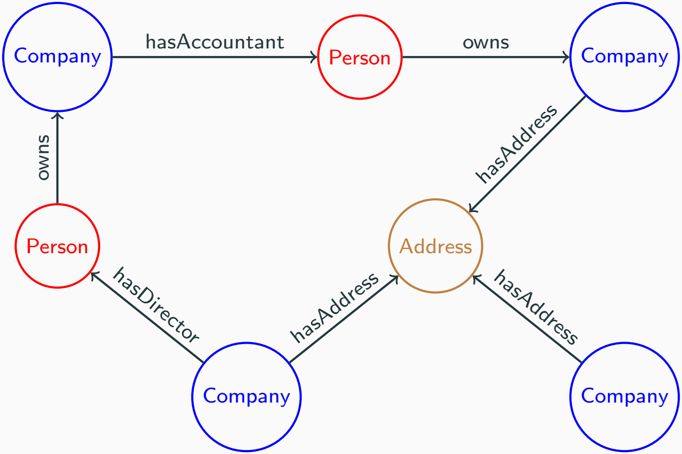
The lab has access to data from other authorities, like data about VAT, tax and income.

Application: Fraud detection

Most of our data is organised in a Neo4j graph database.



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So far we have been using manually curated graph features in our machine learning models.

Application: Fraud detection

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We are currently in the process of implementing graph neural networks to automate this, and (hopefully!) improve the performance of the models as well.

The End

Thank you for your attention.