Graph Neural Networks

Introduction - Part 2

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VIRTUTE ET SAPIENTIA

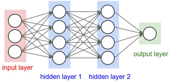
Bitdefender®

May 2021

Choose your model

UNSTRUCTURED

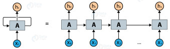
Sepal length	Sepal width	Petal length	Petal width	Species
5.1	3.5	1.4	0.2	Iris setosa
4.9	3.0	1.4	0.2	Iris setosa
7.0	3.2	4.7	1.4	Iris versicolor
6.4	3.2	4.5	1.5	Iris versicolor
6.3	3.3	6.0	2.5	Iris virginica
5.8	3.3	6.0	2.5	Iris virginica



MLP

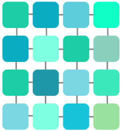
SEQUENTIAL

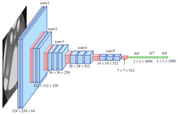
Have a nice day! :)



RNN

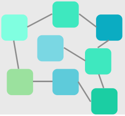
GRID

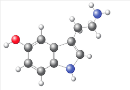


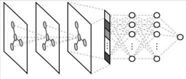


CNN

RELATIONAL STRUCTURE

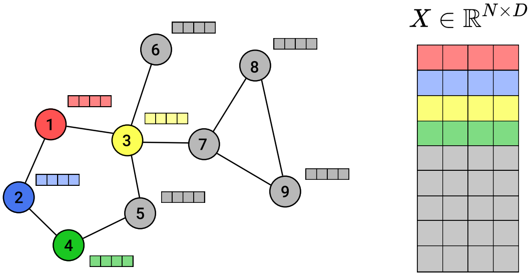






GNN

Graph Data



- all the nodes $x_i \in \mathbb{R}^D$ are stacked into a matrix $X \in \mathbb{R}^{N \times D}$
- each row corresponds to a node $x_i \in \mathbb{R}^D$

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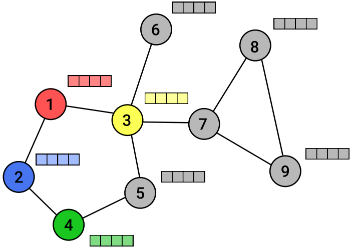
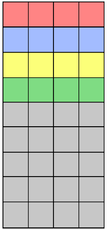


$X \in \mathbb{R}^{N \times D}$



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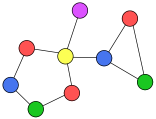
$f\Big($  $\Big) = Y$

Learning

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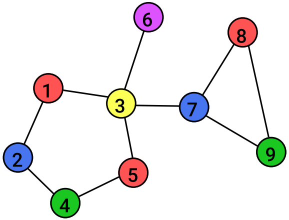
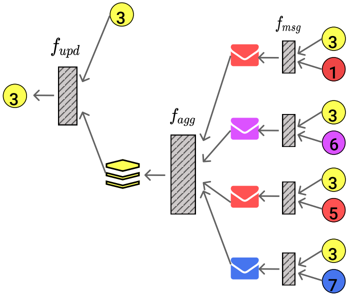
- the output of a GNN for a node i is obtained by applying a **sequence of operations** on the initial nodes
- all the operations along the sequence should be **differentiable**





GNNs: Message Passing Framework - Send

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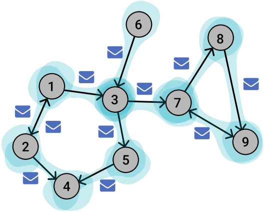

- f_{msg} is a learnable function (e.g. an MLP)
- its parameters are shared between each pair of nodes

$$m_{ij} = \overbrace{f_{msg}(x_i, x_j)}^{\text{Learnable funcion}} \in \mathbb{R}^C \quad \forall (i,j) \in \mathcal{E}$$

$$m_{3,6} = f_{msg}(\quad , \quad)$$

$$m_{3,1} = f_{msg}(\quad , \quad)$$

Same parameters

$$\dots$$

$$m_{4,2} = f_{msg}(\quad , \quad)$$

GNNs: Message Passing Framework - Aggregation

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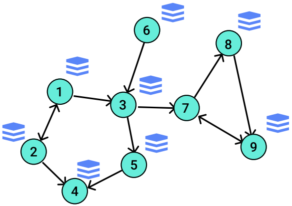


- aggregate incoming messages with the function f_{agg}:
  - usualy not learnable: eg. sum, mean, max, min
  - learnable: e.g. LSTM
- it should be **invariant to the order** of the nodes and should **allow a variable number** of messages

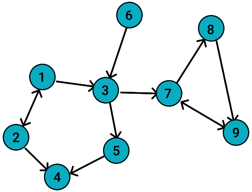
$$h_i = \overbrace{f_{agg}}^{\text{operator}}(\{m_{ij} | \forall j \in \mathcal{N}_i\}) \in \mathbb{R}^C$$

$$h_3 = f_{agg}(\{\text{✉}, \text{✉}\})$$

$$\dots$$

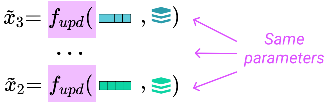
$$h_1 = f_{agg}(\{\text{✉}\})$$

GNNs: Message Passing Framework - Update



- f_{upd} is a learnable function (e.g. an MLP)
- its parameters are shared between all the nodes

$$\tilde{x}_i = \overbrace{f_{upd}(x_i, h_i)}^{\text{Learnable function}} \in \mathbb{R}^C$$



GNNs - Overview

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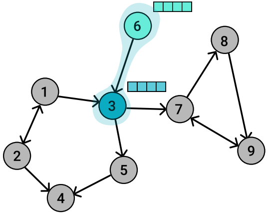
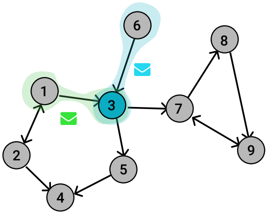
1. Send

$$m_{ij} = f_{msg}(x_i, x_j)$$



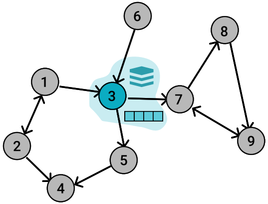
2. Aggregate

$$H_i = f_{agg}(\{m_{ij} | \forall j \in \mathcal{N}_i\})$$



3. Update

$$\tilde{x}_i = f_{upd}(x_i, H_i)$$



Multiple Layers

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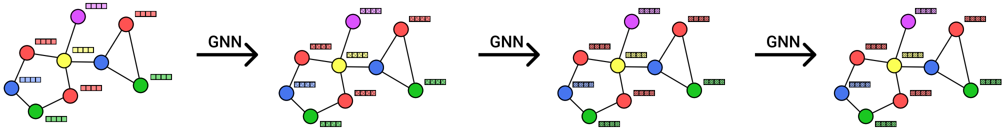
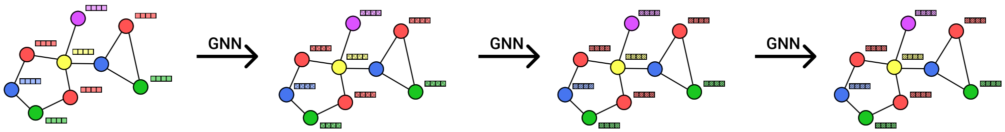
- for a more powerful representation, we can stack multiple layers



Multiple Layers

- for a more powerful representation, we can stack multiple layers
- each layer increases the receptive field of each node



RECEPTIVE FIELD:

Application: Fake News Identification

Goal: determine if a Tweet links to a fake news article

[redacted]

New paper from Brain Zurich and Berlin!

We try a conv and attention free vision architecture: MLP-Mixer (arxiv.org/abs/2105.01601)

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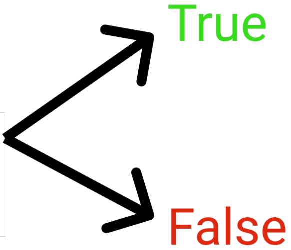

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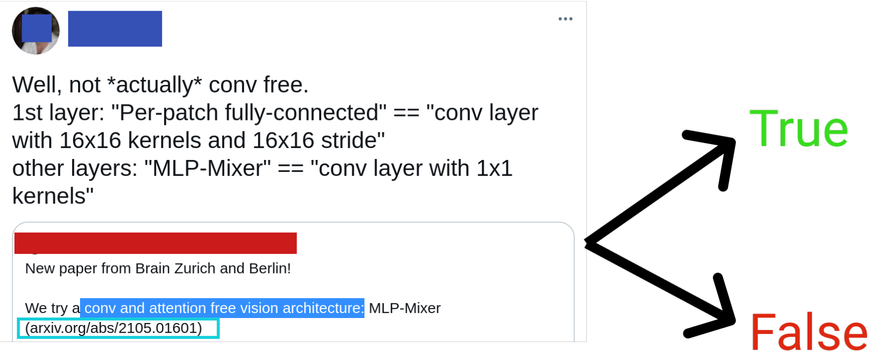

Application: Fake News Identification

Bitdefender

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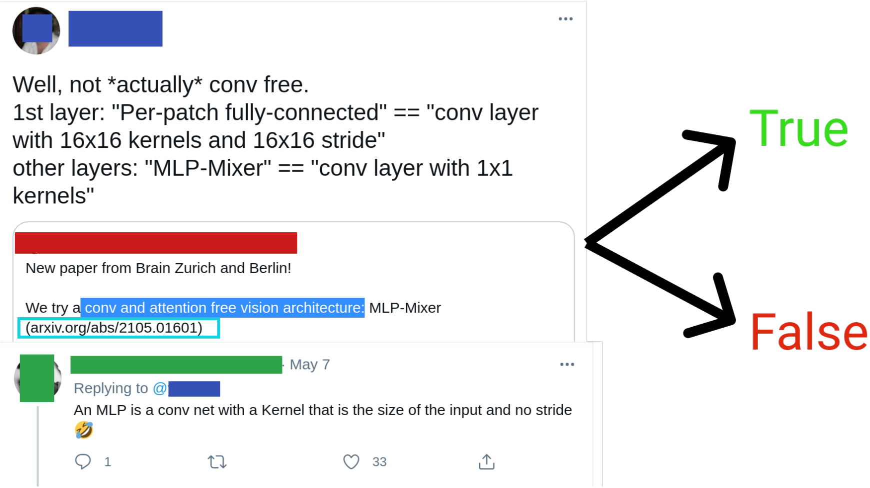

Application: Fake News Identification

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Challenges:

- understanding news requires knowledge of political / social context
- often written in bad faith to appear real
- highly nuanced

[1][1]: Vosoughi et. al. The spread of true and false news online. Science (2018).

Application: Fake News Identification

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News Spread

"Falsehood diffused significantly *farther, faster, deeper, and more broadly* than the truth"[1]

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News Spread

"Falsehood diffused significantly *farther, faster, deeper, and more broadly* than the truth"[1]

Idea

- Analyse the news diffusion patterns with GNNs.

[1] [1]: Vosoughi et. al. The spread of true and false news online. Science (2018).

Application: Fake News Identification

Bitdefender

- gather stories classified by fact-checking orgs like Snopes, PolitiFact
- for each story form a graph of all the tweets and retweets mentioning it
- edges are follow relations or retweet relations

[2]: Monti et. al. Fake news detection on social media using geometric deep learning (2019).

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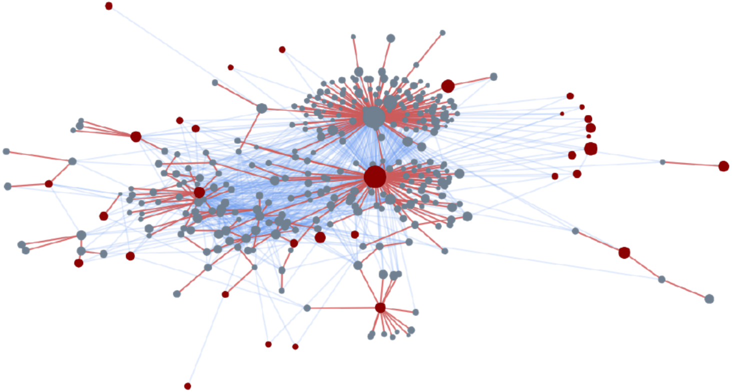

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Application: Fake News Identification

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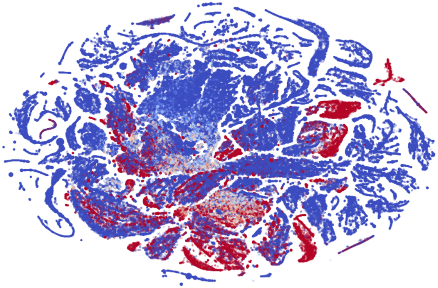
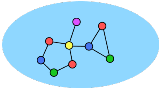
- apply standard GNN model
- node features:
  - User profile (geolocalization, language, embedding of self-description, date of account creation)
  - Network and spreading (No. of followers, timestamps, No. of replies, quotes, favorites and retweets for the source tweet)
  - Content (embeddings of tweet text).
    - Surprising: not that relevant!

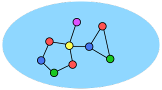


When to use GNNs?



- What are the cases where it is beneficial to use GNNs? 

When to use GNNs?



- What are the cases where it is beneficial to use GNNs?
- What design choices should be made for a specific task?
    - Do we want sum or max in the aggregation?
    - Should we share parameters between layers?
    - Should we use distances or order information when we have them?

When to use GNNs?

Bitdefender

Usual deep Learning approach:

- learn end-to-end $f(X)$ from data with the specific model f (MLP, CNN, RNN etc.)
- each model is appropriate in certain cases

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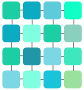
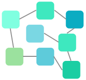
Inductive biases

An inductive bias allows a learning algorithm to prioritize one solution over another, independent of the observed data.

	UNSTRUCTURED	SEQUENTIAL	GRID	COMPLEX RELATIONAL STRUCTURE
Structure				
Model	MLP	RNN	CNN	GNN
Inductive Bias	Weak	Sequentiality	Locality	Strong relational bias

Relational Reasoning

Bitdefender

Relational Reasoning

Manipulating *structured* data, that consists in multiple **entities** that establish various **relations** between them.

Relational Reasoning

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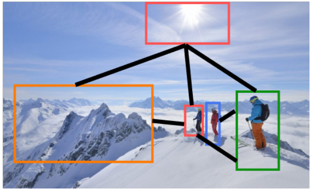
Manipulating *structured* data, that consists in multiple **entities** that establish various **relations** between them.

From some perspective, relational reasoning could be appealing.
For example, a visual scene could be seen as:

- an image / a grid of points
- a set of objects with multiple relations between them



Relational Inductive Biases

Bitdefender

Inductive biases
An inductive bias allows a learning algorithm to prioritize one solution over another, independent of the observed data.

Relational inductive biases in GNN:

- explicit factorisation into nodes, each corresponding to an entity
- explicit modeling of pairwise relations between nodes
- flexibility in establishing different connectivity
- order invariant

[3] Battaglia et. al. Relational inductive biases, deep learning, and graph networks. 2018

When to use a GNN?

Bitdefender

GNNs could be appropiate if:

- there exist entities and relations in the data
    - explicit: social networks, molecules
    - implicit: visual scenes, environments...
- the relational processing is beneficial

Shortest path Problem

Bitdefender

- Lets analyse a purely reasoning problem of finding the shortest path in a graph.
  - Can GNNs solve this problem and how sample efficient are they?

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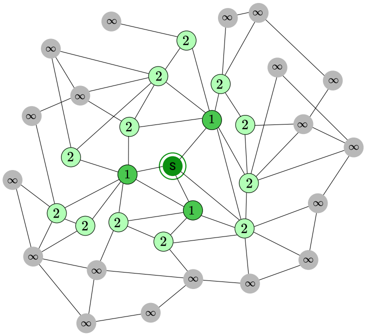

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GNN Method

for layer k in 1 .. K **do**
  for node i in $\mathcal{V}$ **do**
    $$x_i^k = f_{upd}\{x_i^{k-1}, \underset{\forall j \in \mathcal{N}_i}{f_{agg}} \{f_{msg}(x_i^{k-1}, x_j^{k-1})\}$$
  end for
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	for iter k in 1 .. K **do**
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Task Alignment

Bitdefender

- if the GNN learns to simulate the update step in the Dynamic Problem, it will solve the problem
- if the operation is easy to lean, then the GNN can easily solve the problem
- if both are true, we say that the GNN is *well aligned* with the task

[4] Xu et. al. What Can Neural Networks Reason About? ICLR 2020

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Alignment

We say that a model is **aligned** with a task, if by replacing some parts of the model with some ideal operations we would solve the task. If the parts can *easily learn* the ideal operations, we say that it is **well aligned** with the task.

Generally:

- If a model is well aligned with a task, it will lean it easily (it has low sample complexity).

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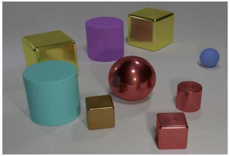
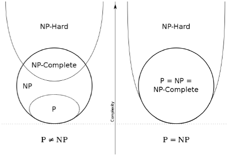
- What decision can we take to have the GNN "more aligned"?
    - use **min** as an aggregator function
    - **share** the parameters between layers
- Is $\tilde{x}_i = \text{MLP}([x_1, x_2, ...x_N])$ well aligned?
    - it is less aligned than the GNN functions
    - it has to learn to create node pairs and then it has to select the minimum between

Alignment

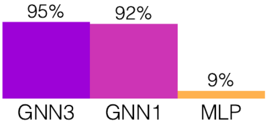


Relational argmax
What are the colors of the furthest pair of objects?

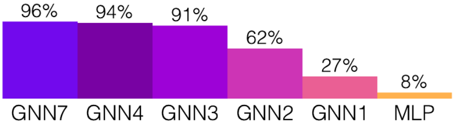
Dynamic programming
What is the cost to defeat monster X by following the optimal path?



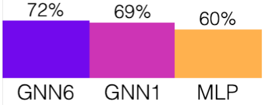
NP-hard problem
Subset sum: Is there a subset that sums to 0?



Relational argmax



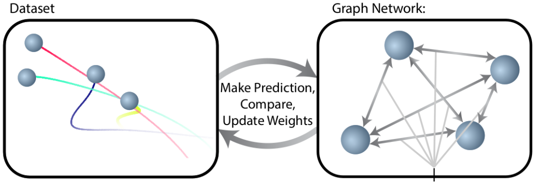
Dynamic Programming



NP - hard problem (random = 50%)

Alignment: Physical Particles

Bitdefender



GNNs	Analogy to Newtonian Mechanics
Nodes	Particles
Pair of nodes	Two interacting particles (i,j)
Send Function: f_{msg}	Compute force F_{ij}
Aggregate Function: f_{msg}	Sum into net force $F_{net,i}$
Update Function: f_{msg}	Compute acceleration $a_i = F_{net,i}/m_i$

[5]: Cranmer et. al. Discovering Symbolic Models from Deep Learning with Inductive Biases. Neurips 2020.

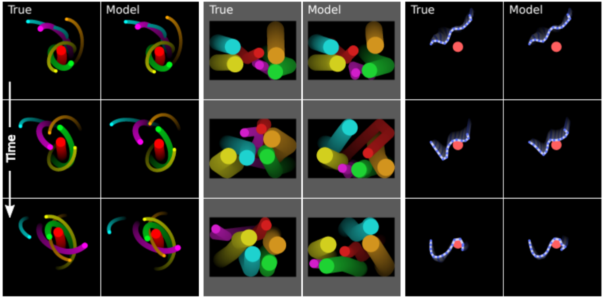
When to use a GNN?

- Apply GNNs on tasks that are well aligned with this model
  - dynamic programming
  - relational reasoning
- Apply GNNs when relational processing is beneficial
  - explicit entities and relations: social networks, molecules
  - implicit entities and relations: visual scenes, environments...
- Try to design your GNN to be as aligned as possible to your problem

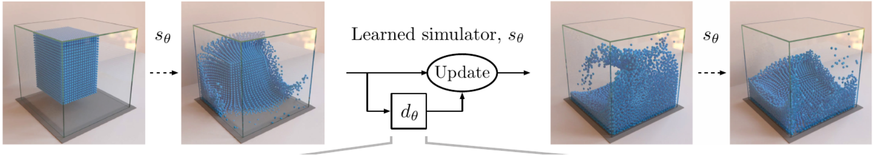
Application: Physical Particle Interactions

Bitdefender

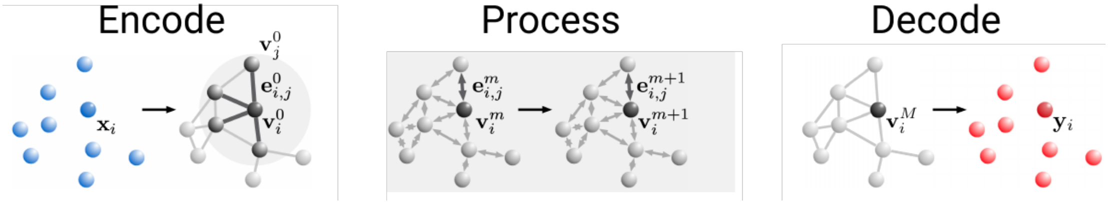
[6] Battaglia et. al. NeurIPS 2016



[7] Gonzalez et al. ICML 2020



Application: Physical Particle Interactions

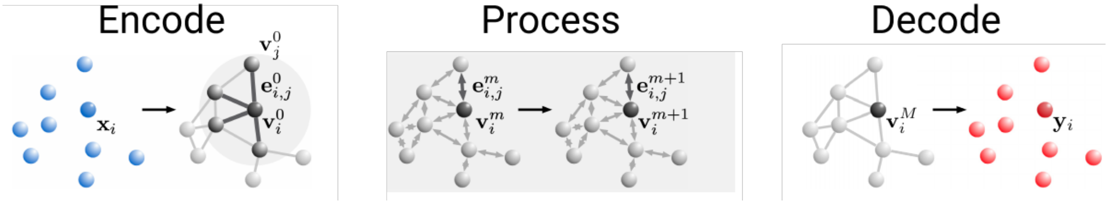


Encoder:

- each node corresponds to a particle
- link top-k nearest neighbors
- Node features:
    - position and velocity
    - particle type

[7] Gonzalez et al. ICML 2020

Application: Physical Particle Interactions



Process:

- use 10 GNN layers
- local propagation based on neighbourhood

Decoder:

- predict next step attributes
- train based on node level loss

[7] Gonzalez et al. ICML 2020

Application: Physical Particle Interactions

Bitdefender

Observations:

- the method is traned for next step predictions but at test time is unrolled for thousand of steps
- GNN method could generalise to 34 times more nodes at test time
  - because the interactions to nearest neighbours
- relative positions are is better than global positions
  - underlying physical processes are invariant to spatial position,

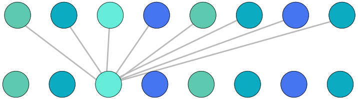
Overall:

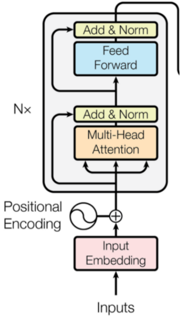
- GNN is aligned to the task
- the GNN has built in good relational biases
  - use local interactions
  - relative position for built in spatial invariance

Transformer

Bitdefender

Task: analyse a sequence of words. $X = x_1, x_2, ..., x_N$.





Transformer

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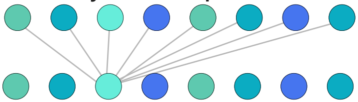
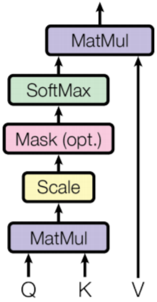


Scaled Dot-Product Attention



Self - Attention

- Process a sequence in multiple layers
- Each element attends to all other elements in the previous layer

$$Y = \text{softmax}(\frac{QK^T}{\sqrt{d}})V$$

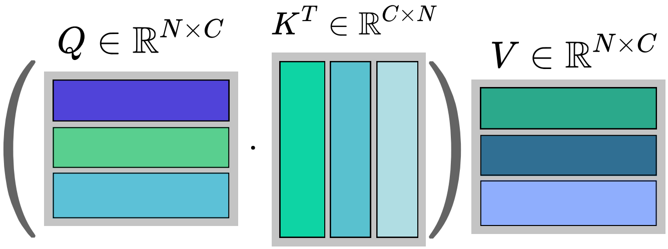
- where $Q = XW_q, K = XW_k, V = XW_v$

Transformer

Self-attention

$$Y = \text{softmax}(\frac{QK^T}{\sqrt{d}})V$$

where $Q = XW_q, K = XW_k, V = XW_v$



Transformer

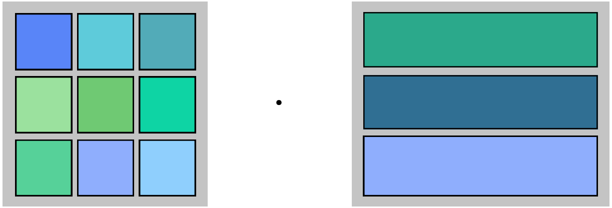
Bitdefender

Self-attention

$$Y = \text{softmax}(\frac{QK^T}{\sqrt{d}})V$$

where $Q = XW_q, K = XW_k, V = XW_v$

$A \in \mathbb{R}^{N \times N}$ $\qquad$ $V \in \mathbb{R}^{N \times C}$



Transformer

Self-attention

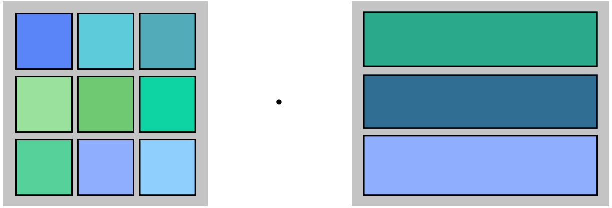
$$Y = \underbrace{\text{softmax}\left(\frac{QK^T}{\sqrt{d}}\right)}_{\boxed{A}} V$$

GCN

$$Y = \sigma(\boxed{A}\,\boxed{XW})$$

where $Q = XW_q$, $K = XW_k$, $\boxed{V = XW_v}$

$A \in \mathbb{R}^{N \times N}$ $\quad$ $V \in \mathbb{R}^{N \times C}$



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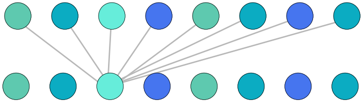
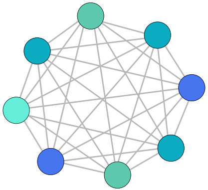


$$Y = \frac{QK^T}{\sqrt{d}}V$$

$$y_i = \sum_{\forall j} \underbrace{\frac{1}{\sqrt{d}} \overbrace{(x_i W_q)}^{\text{Query}} \overbrace{(x_j W_k)^T}^{\text{Key}}}_{\alpha(x_i,x_j)} \overbrace{(x_j W_v)}^{\text{Value}}$$



$$y_i = f_{upd}(x_i, \sum_{\forall j \in \mathcal{N}_i} \{\alpha(x_i, x_j)\phi(x_j)\})$$

$$\alpha(x_i, x_j) = \frac{1}{\sqrt{d}}(x_i W_q)^T (x_j W_k)$$

$$\phi(x_j) = x_j W_j$$

Transformer

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Transformers vs GNNs

Transformer is a special case of Graph Neural Networks where

- all the nodes are connected
- pairwise messages are weighted by dot product attention

Transformer - NLP

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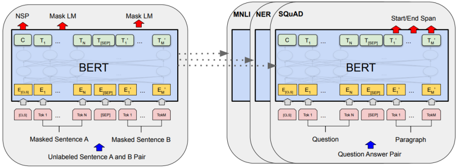
Transformers are now the standard model in NLP.

BERT [8]



Pre-training

Fine-Tuning

GPT-3 [9]

Zero-shot

The model predicts the answer given only a natural language description of the task. No gradient updates are performed.

```
Translate English to French:     ← task description
cheese =>                        ← prompt
```

One-shot

In addition to the task description, the model sees a single example of the task. No gradient updates are performed.

```
Translate English to French:     ← task description
sea otter => loutre de mer       ← example
cheese =>                        ← prompt
```

Transformer - Vision

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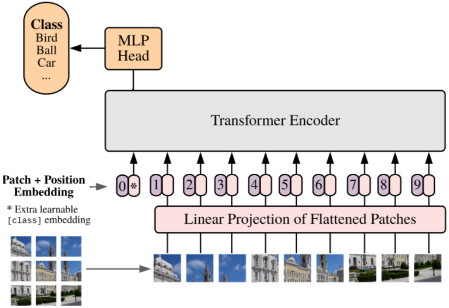
Transformers are becoming popular in CV.

ViT [10]



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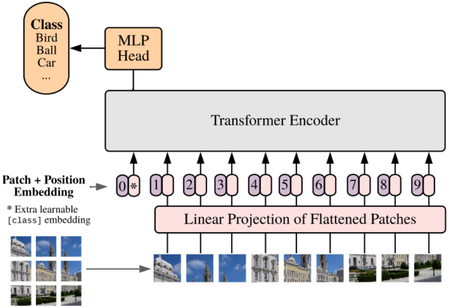
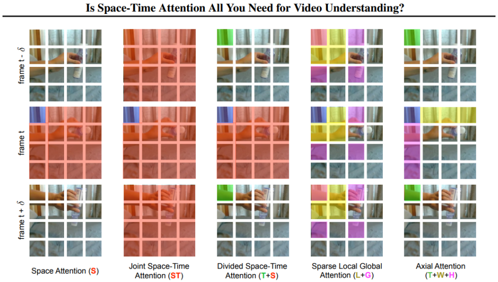


TimeSformer [11]



GNN - Challenges: Scalability

Context:

- ML methods work with mini-batches where each element is independent

- in many *node level* graph tasks, the entire dataset forms a large graph where each node is connected to many other ones.

Problem:

- the whole graph is too big to fit into memory.

    - process independently the neighbourhood of each node

    - the neighbourhood could still grow exponentially:

Challenges: Scalability

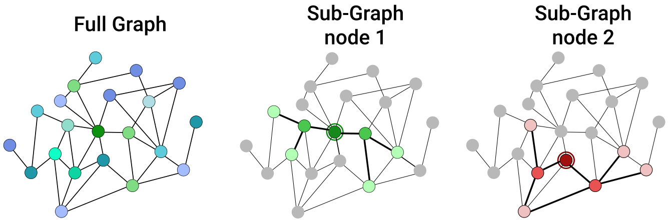
Bitdefender

Solution:

- sample [12],[13] the nodes, forming sub-graphs and apply the GNN over them

Benefits:

- can work with very large graphs
- the sampling acts as a regularizer, similar to dropout

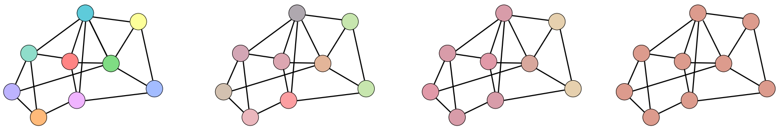


Challenges: Oversmoothing

Bitdefender

If we want node information from a K-order neighbourhood

- use K layers of Graph propagation
- usual problems
  - harder to optimize due to vanishing / exploding gradients
  - overfitting due to large number of parameters
- graph propagation problem: **oversmoothing**
  - graph propagation can be seens as "smoothing" the a node according to its neighbourhood
  - if we do many propagations, different nodes would become almost *indistinguishable*, hurting *node-level* tasks



Challenges: Oversmoothing

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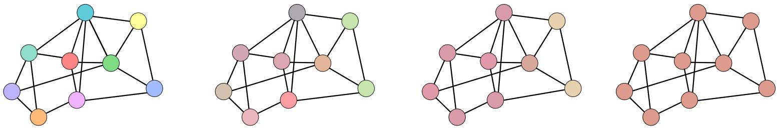
Oversmoothing
Nodes with similar structure in their neighbourhoods would end up indistinguishable, regardless of their initial features.

More often:

- when the graph is dense
- when using self-loop in the update function

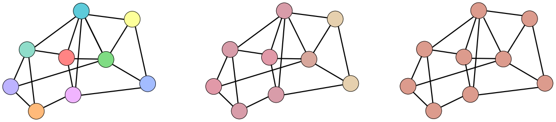


Oversmoothing: Solutions

Bitdefender

Solutions:

- **residual** Connections [14, 15]:
    - skip one or more layers
    - add the representations of a node from different layers $h_i^{k+1} \leftarrow h_i^{k+1} + h_i^k$
    - takes more into account the identity of each node



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Bitdefender

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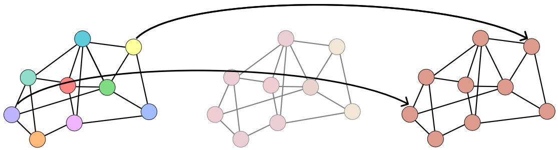

Oversmoothing: Solutions

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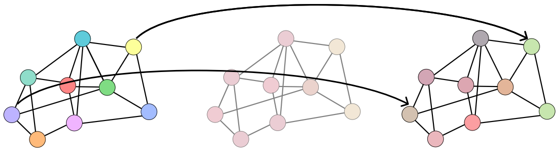

Oversmoothing: Solutions

Bitdefender

Solutions:

- make the graph more **sparse**: e.g apply dropout on edges [16]

- PairNorm[17]: add a **normalisation** term that encourages h_i^{t+1} and h_i^t to remain close while neighbouring nodes maximise their similarity and distant does minimise their similarity

Connections to PageRank

Bitdefender

Long range are obtained by stacking multiple layers: $A\sigma(A..\sigma(AXW_1)..W_{n-1})W_n$

Connections to PageRank

Bitdefender

Long range are obtained by stacking multiple layers: $A\sigma(A..\sigma(AXW_1)..W_{n-1})W_n$

Random Walk

- start in a node and randomly move to adjacency nodes.
- $W = I$ and $X \in \mathbb{R}^N$ a vector containing the probability of being in each node and A is the transition probability
- this arrives at the PageRank algorithm $X^{t+1} = AX^t$

Connections to Personalised PageRank

- PageRank converges to an Y that does not depend of the initial X
- this is related to the oversmoothing problem in the GNN
- in Personalised PageRank the initial starting point count more
  - at each step there is a chance α to go back to the initial state $X^{t+1} = (1-\alpha)AX^t + \alpha X^0$

Connections to Personalised PageRank

Bitdefender

- PageRank converges to an Y that does not depend of the initial X
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- in Personalised PageRank the initial starting point count more
  - at each step there is a chance α to go back to the initial state $X^{t+1} = (1-\alpha)AX^t + \alpha X^0$
- we can use a similar formulation in our graph propagation to alleviate the oversmoothing
  - the residual connection could be seen as a non-probabilistic variant

Connections to Personalised PageRank

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How can it be used in GNNs?

- make a prediction independently at each node and propagate the answer [18]

$$X^1 = X^0 W$$
$$X^{t+1} = (1-\alpha) A X^t + \alpha X^0$$

Connections to Personalised PageRank

How can it be used in GNNs?

- make a prediction independently at each node and propagate the answer [18]

$$X^1 = X^0 W$$
$$X^{t+1} = (1-\alpha) A X^t + \alpha X^0$$

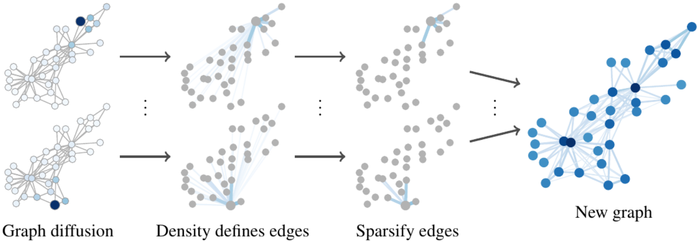
- this is somehow related to label propagation [19]

Connections to Personalised PageRank

Alternatively:

- compute Personalized Page Rank diffusion matrix S [20][21]
- sparsify the diffusion matrix
- and use it in a GCN

$$Y = \sigma(SXW)$$



Overview

- Graph Neural Network framework

Overview

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- Graph Neural Network framework
- application: fake news detection

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- When to use GNNs?
  - relational inductive biases
  - alignment

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Overview

Bitdefender

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- challenges: oversmoothing
- connections to PageRank

Graph Neural Networks - Resources

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For a more in depth understanding of Graph Neural Networks and other related areas, please take a look:

- Michael Bronstein, *Geometric deep learning, from Euclid to drug design* Link
- Petar Veličković, *Theoretical Foundations of Graph Neural Networks* Link
- Jure Leskovec, *CS224W: Machine Learning with Graphs* Link
- William L. Hamilton, *Graph Representation Learning Book* Link
- Razvan Pascanu, *GraphNets - Lecture at TMLSS (Transylvanian Machine Learning Summer School)*
- Xavier Bresson, *Convolutional Neural Networks on Graphs* Link
- Michael Bronstein, *Graph Deep Learning Blog* Link

Thank You!

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May 2021

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