

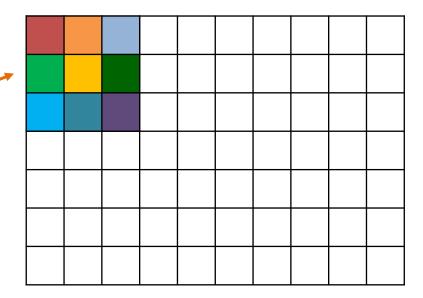
# Deep Learning on graphs

Prof. Leal-Taixé and Prof. Niessner

#### The domain so far

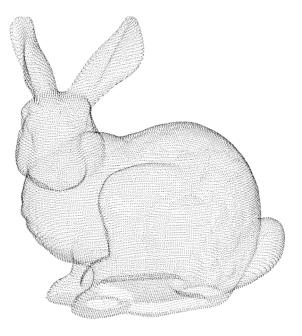
- Regularity on the domain
  - Order of the pixels is important

Your convolution filter imposes a certain structure



#### A new domain

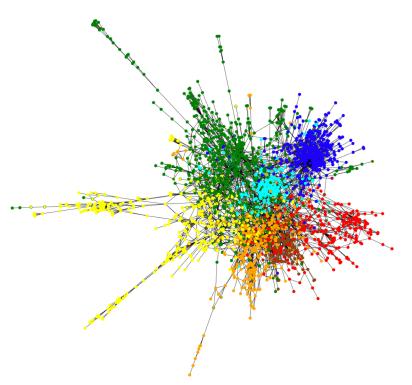
- Rich Information
  - 3D Point Location
  - Other features:
    - RGB/ Intensity
    - Semantic
- Irregularity
  - Permutation Invariance
  - Transformation Invariance



#### Point Cloud

#### A new domain

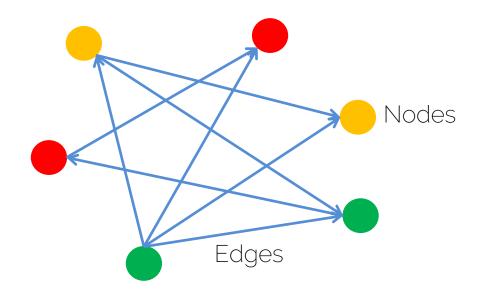
- A citation network
  - Each node is a paper
  - Connection is a citation
- Similar for:
  - Social networks
  - Recommender systems



M. Bronstein et al. "Geometric deep learning: going beyond Euclidean data". IEEE Signal Processing Magazine. 2017

# A graph

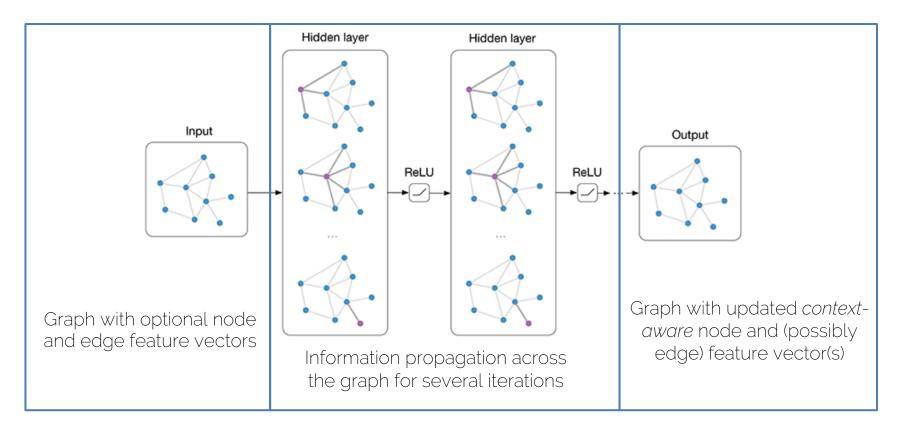
- Node: a concept
- Edge: a connection between concepts



# Deep learning on graphs

- Generalizations of neural networks that can operate on graph-structured domains:
  - Scarselli et al. "The Graph Neural Network Model". IEEE Trans. Neur. Net 2009.
  - Kipf et al. "Semi-Supervised Classification with Graph Convolutional Networks. ICLR 2016.
  - Gilmer et al. "Neural Message Passing for Quantum Chemistry". ICML 2017
  - Battaglia et al. "Relational inductive biases, deep learning, and graph networks". arXiv 2018 (review paper)
- Key challenges:
  - Variable sized inputs (number of nodes and edges)
  - Need invariance to node permutations

#### General Idea

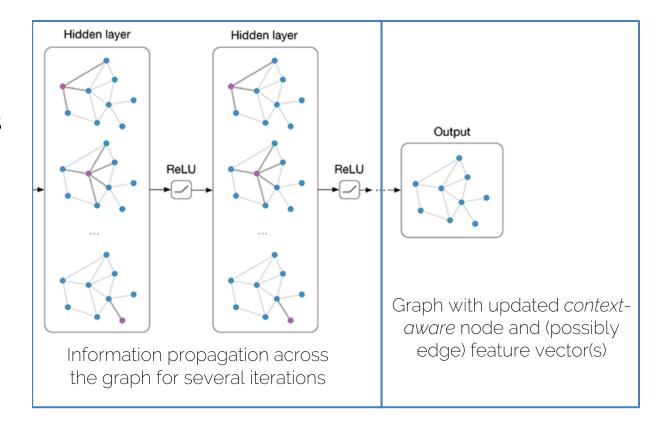


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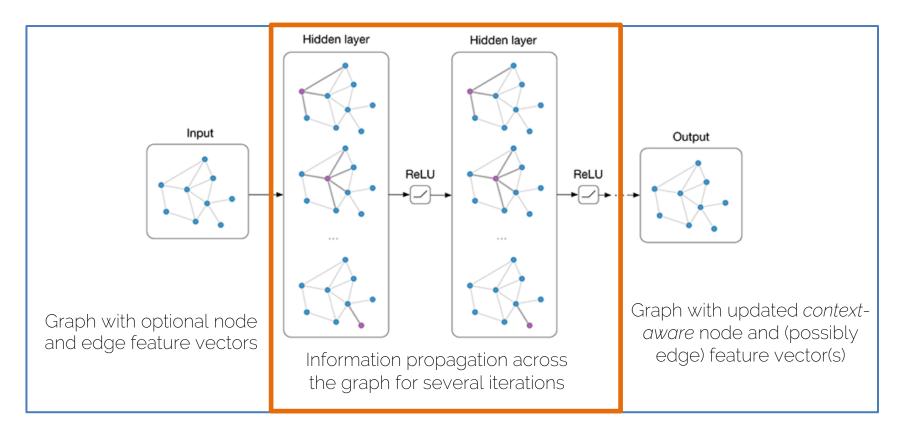
Figure credit: <u>https://tkipf.github.io/graph-convolutional-networks/</u>

#### General Idea

Each update step is understood as a "layer" in common NNs

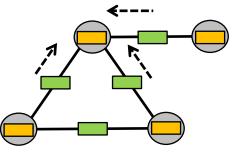


#### General Idea



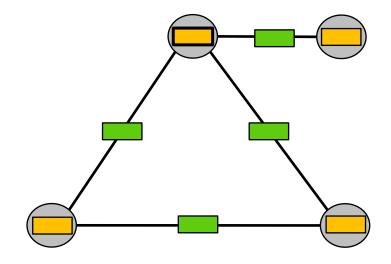
- Notation:

  - Graph: G = (V, E)- Initial embeddings:  $h_{(i,j)}^{(0)}, (i,j) \in E$   $h_i^{(0)}, i \in V$  Node embeddings after l steps:  $h_i^{(l)}, i \in V$
- Goal:
  - Encode contextual graph information in node embeddings by iteratively combining neighboring nodes' features





- At every iteration, every node receives features from its neighboring nodes.
- These features are then aggregated with an order invariant operation and combined with the current features with a learnable function



- At every message passing step l , for every node do:

$$m_v^{(l+1)} = \sum_{u \in N_v} M^{(l)}(h_u^{(l)}, h_v^{(l)}, h_{(u,v)}^{(0)})$$
Message Learnable function (e.g. MLP) with shared weights across the entire graph

Aggregation overall all neighbors

- At every message passing step l , for every node do:

$$m_v^{(l+1)} = \sum_{u \in N_v} M^{(l)}(h_u^{(l)}, h_v^{(l)}, h_{(u,v)}^{(0)})$$

$$h_v^{(l+1)} = U^{(l)}(h_v^{(l)}, m_v^{(l+1)})$$

Embedding update

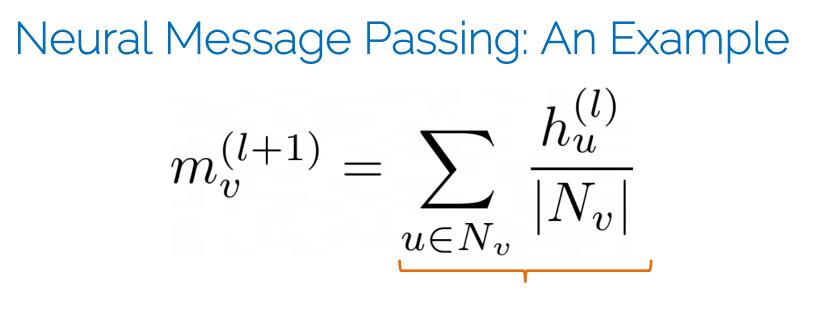
Learnable function (e.g. MLP) with shared weights across the entire graph

- At every message passing step l , for every node do:

$$m_v^{(l+1)} = \sum_{u \in N_v} M^{(l)}(h_u^{(l)}, h_v^{(l)}, h_{(u,v)}^{(0)})$$

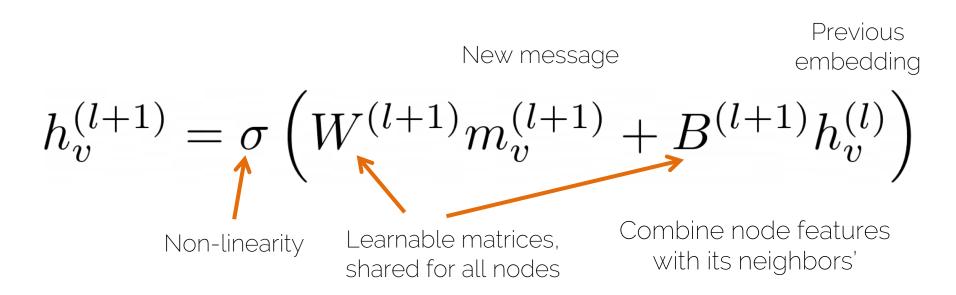
$$h_v^{(l+1)} = U^{(l)}(h_v^{(l)}, m_v^{(l+1)})$$

Most Graph Neural Network Models can be seen as specific example of this formulation



Average neighbors' feature embeddings

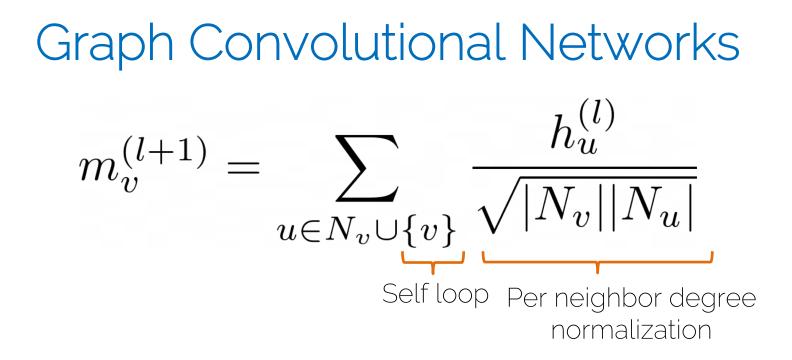
#### Neural Message Passing: An Example



#### Neural Message Passing: An Example

- We can use MLPs or even recurrent networks, instead of linear functions
- These are THE SAME for ALL nodes and edges!

$$h_v^{(l+1)} = \sigma \left( MLP_1^{(l+1)} m_v^{(l+1)} + MLP_2^{(l+1)} h_v^{(l)} \right)$$



$$\begin{aligned} & \text{Graph Convolutional Networks} \\ & m_v^{(l+1)} = \sum_{u \in N_v \cup \{v\}} \frac{h_u^{(l)}}{\sqrt{|N_v||N_u|}} \\ & h_v^{(l+1)} = \sigma \left( W^{(l+1)} m_v^{(l+1)} \right) \end{aligned}$$

Same learnable matrix for self-loops and regular neighbors

$$\begin{aligned} & \text{Graph Convolutional Networks} \\ & m_v^{(l+1)} = \sum_{u \in N_v \cup \{v\}} \frac{h_u^{(l)}}{\sqrt{|N_v||N_u|}} \\ & h_v^{(l+1)} = \sigma \left( W^{(l+1)} m_v^{(l+1)} \right) \end{aligned}$$

Matrix of weights is of size = #channels out x #channels in

### Graph Convolutional Networks

• We want to collect information from our neighbors and convert it to a new embedding

$$h_v^{(l+1)} = \sigma\left(W^{(l+1)}m_v^{(l+1)}\right)$$

Matrix of weights is of size = #channels out x #channels in

Graph Convolutional Networks
$$m_v^{(l+1)} = \sum_{u \in N_v \cup \{v\}} \frac{h_u^{(l)}}{\sqrt{|N_v||N_u|}}$$

• Unlike a normal image convolutional filter, here the neighbors are not regular (as they are in the image space), hence I have to do a permutation-invariant aggregation operation before the convolution.

Graph Convolutional Networks  

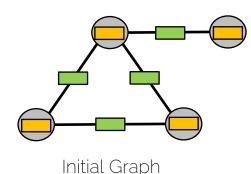
$$m_{v}^{(l+1)} = \sum_{u \in N_{v} \cup \{v\}} \frac{h_{u}^{(l)}}{\sqrt{|N_{v}||N_{u}|}}$$
Aggregation
$$h_{v}^{(l+1)} = \sigma \left( W^{(l+1)} m_{v}^{(l+1)} \right)$$
Convolution

# What About Edge Embeddings?

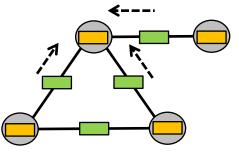
- The framework we've presented is only suited to learn node embeddings. But what happens if our focus is on edge features?
- At least, two options:
  - Work on the 'dual' or 'line' graph
    - E.g. Chen et al. "Supervised Community Detection with Line Graph Neural Networks", ICLR 2019.
  - Use a more general formulation that admits edge updates
    - E.g. Battaglia et al. "Relational inductive biases, deep learning, and graph networks". arXiv 2018

#### A More General Framework

• We can divide the propagation process in two steps: 'node to edge' and 'edge to node' updates.



'Node to edge' Update



'Edge to Node' Update



### 'Node to edge' updates

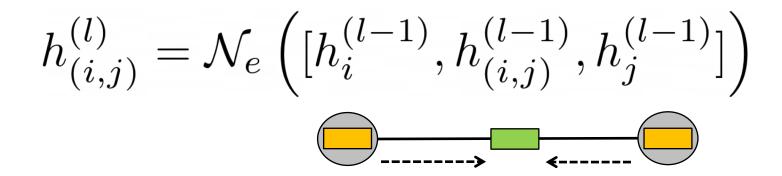
- At every message passing step  $\,l$  , first do:

$$h_{(i,j)}^{(l)} = \mathcal{N}_e\left([h_i^{(l-1)}, h_{(i,j)}^{(l-1)}, h_j^{(l-1)}]\right)$$

Embedding of node i in the precious message passing step Embedding of edge (i,j) in the previous message passing step Embedding of node j in the precious message passing step

### 'Node to edge' updates

- At every message passing step  $\,l$  , first do:

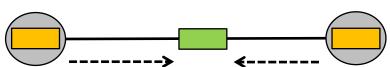


### 'Node to edge' updates

- At every message passing step  $\,l$  , first do:

 $h_{(i,j)}^{(l)} = \mathcal{N}_e\left( [h_i^{(l-1)}, h_{(i,j)}^{(l-1)}, h_j^{(l-1)}] \right)$ 

Learnable function (e.g. MLP) with shared weights across the entire graph

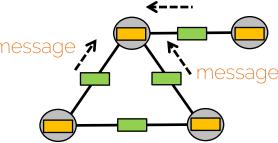


## 'Edge to node' updates

- After a round of edge updates, each edge embedding contains information about its pair of incident nodes
- Then, edge embeddings are used to update nodes:  $m_i^{(l)} = \Phi\left(\left\{h_{(i,j)}^{(l)}\right\}_{j \in N_i}\right)$ message message 🔊 Order invariant Neighbors of message operation (e.g.

sum, mean, max)

node i



# 'Edge to node' updates

- After a round of edge updates, each edge embedding contains information about its pair of incident nodes
- Then, edge embeddings are used to update nodes:

$$m_i^{(l)} = \Phi\left(\left\{h_{(i,j)}^{(l)}\right\}_{j \in N_i}\right)$$
$$h_i^{(l)} = \mathcal{N}_v\left(\left[m_i^{(l)}, h_i^{(l-1)}\right]\right)$$

Learnable function (e.g. MLP) with shared weights across the entire graph

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The aggregation provides each node embedding with contextual information about its neighbors

#### Remarks

- Main goal: obtaining node and edge embeddings that contain *context information* encoding graph topology and neighbor's feature information.
- After repeating the node and edge updates for l steps, each node (resp. edge) embedding contains information about all nodes (resp. edge) at distance l (resp. l − 1) → Think of iterations as layers in a CNN
- Observe that all operations used are differentiable, hence, MPNs can be used within end-to-end pipelines
- There is vast literature on different instantiations, as well as variations of the MPN framework we presented. See Battaglia et al. for an extensive review.



Message Passing Networks for Computer Vision

Prof. Leal-Taixé and Prof. Niessner

# Different challenges

- Multiple objects of the same type
- Heavy occlusions
- Appearance is often very similar





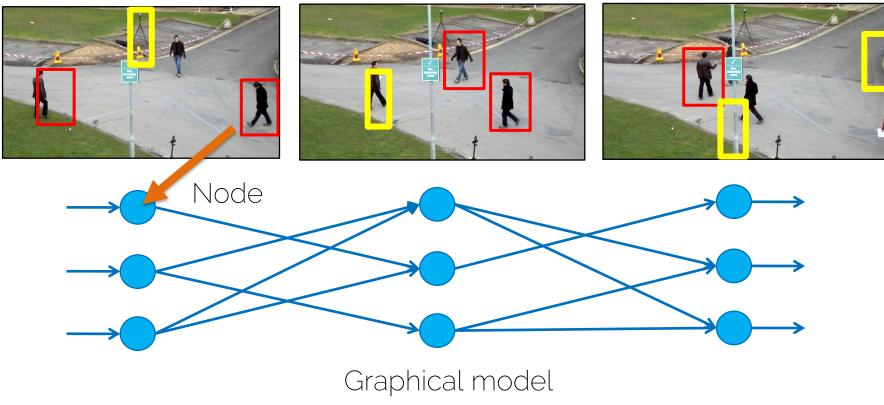
#### Multi-object tracking with graphs



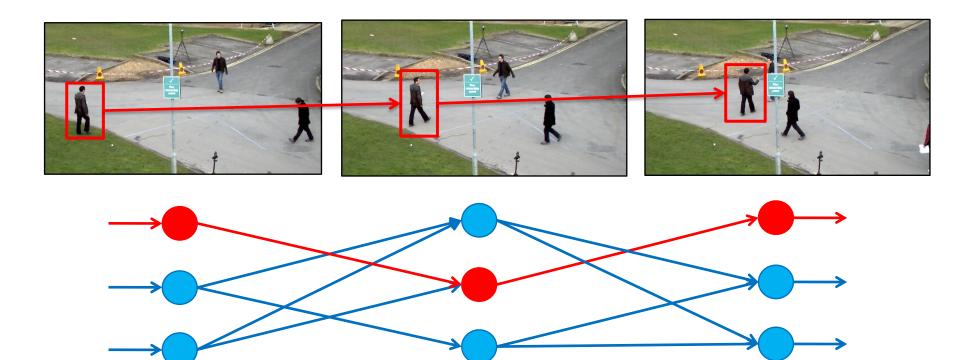
#### Step 1: Object detection

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#### Multi-object tracking with graphs

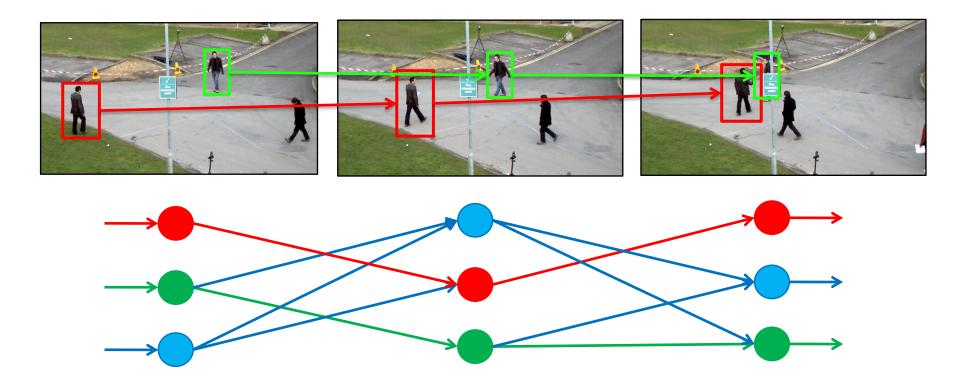


#### Multi-object tracking with graphs



L. Leal-Taixé et al. "Everybody needs somebody: Modeling social and grouping behavior on a linear programming multiple people tracker." ICCVW2011 Prof. Leal-Taixé and Prof. Niessner 36

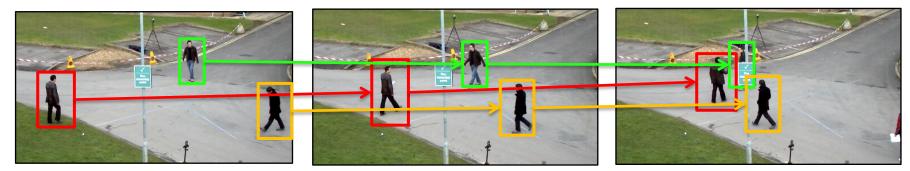
### Multi-object tracking with graphs

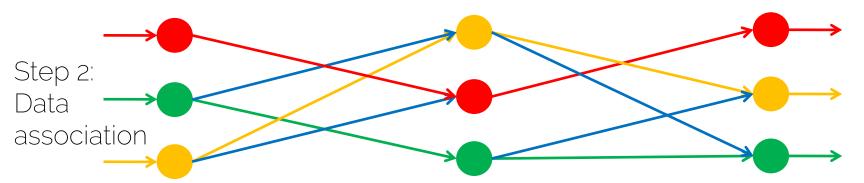


L. Leal-Taixé et al. "Everybody needs somebody: Modeling social and grouping behavior on a linear programming multiple people tracker." ICCVW2011 Prof. Leal-Taixé and Prof. Niessner 37

# Multi-object tracking with graphs

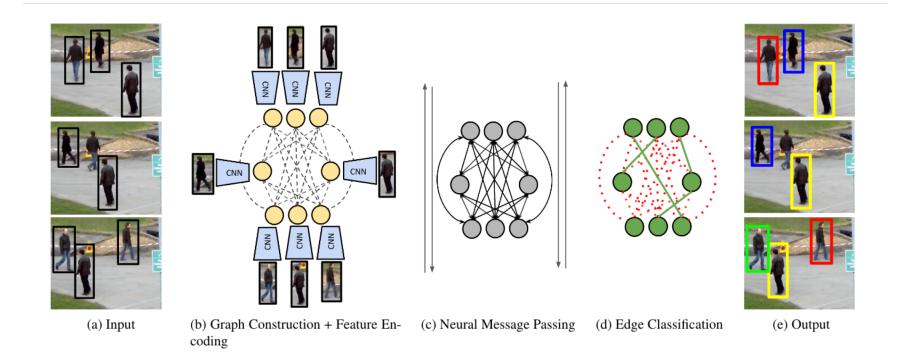
#### Step 1: Object detection





L. Leal-Taixé et al. "Everybody needs somebody: Modeling social and grouping behavior on a linear programming multiple people tracker." ICCVW2011 Prof. Leal-Taixé and Prof. Niessner 38

#### MOT with MPN: Overview

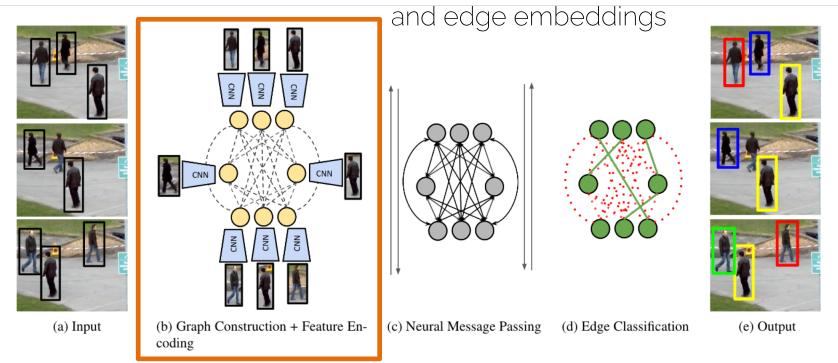


Prof. Leal-Taixé and Prof. Niessner

G. Brasó and L. Leal-Taixé. "Learning a Neural Solver for Multiple Object Tracking", CVPR 2020

### MOT with MPN: Overview

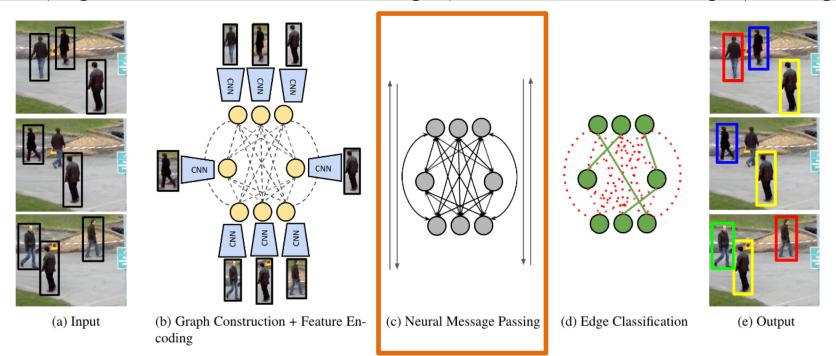
Encode appearance and scene geometry cues into node



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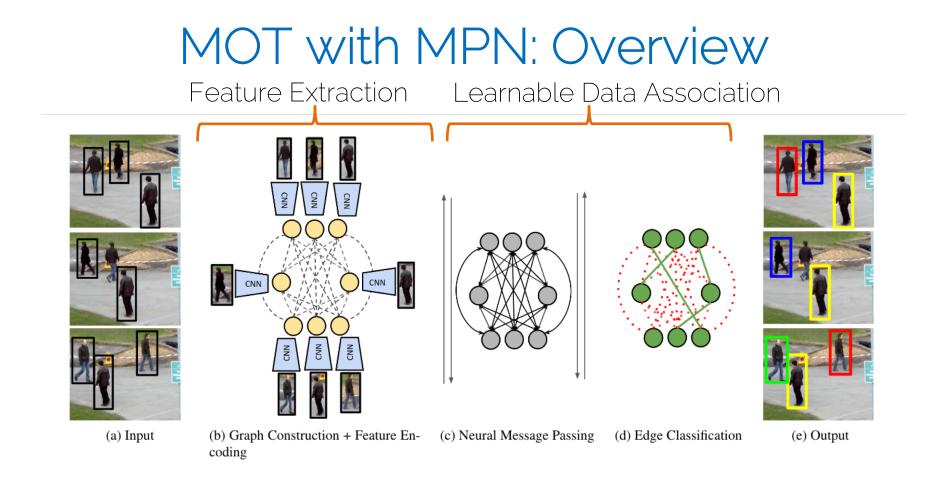
#### MOT with MPN: Overview

Propagate cues across the entire graph with neural message passing

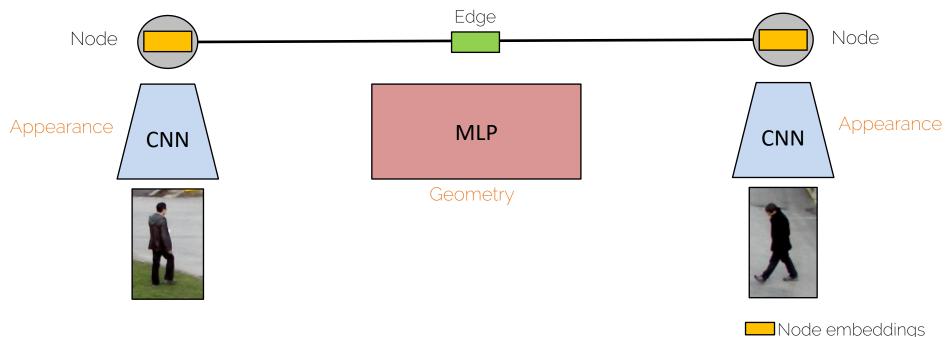


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#### MOT with MPN: Overview Learn to directly predict solutions of the tracking graph problem by classifying edge embeddings (b) Graph Construction + Feature En-(c) Neural Message Passing (d) Edge Classification (e) Output (a) Input coding



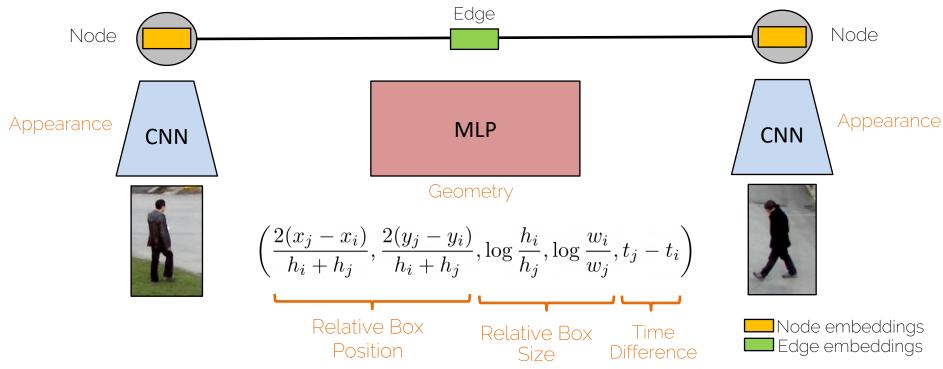
• Appearance and geometry encodings



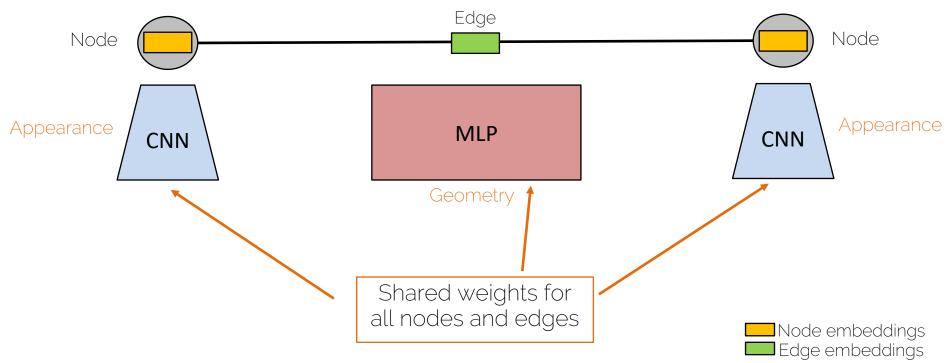
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Edge embeddings

• Appearance and geometry encodings

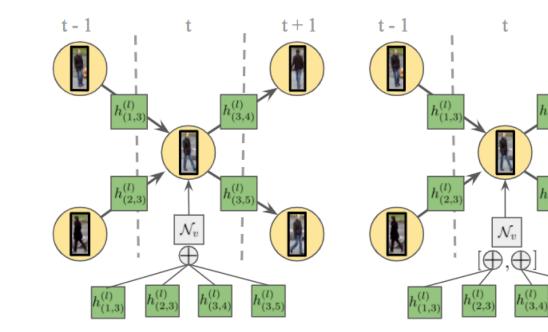


• Appearance and geometry encodings



• Goal: propagate these embeddings across the entire graph in order to obtain new embeddings encoding high-order information among detections

# Time-aware Message Passing



#### All edge embeddings are aggregated at once

Aggregation of edge embeddings is separated between past / future frames

 $h_{(3,...)}^{(l)}$ 

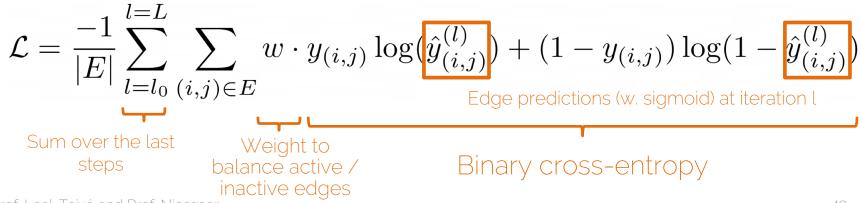
(l)

 $h_{(3,5)}^{(l)}$ 

t + 1

# Classifying edges

- After several iterations of message passing, each edge embedding contains high-order information about other detections
- We feed the embeddings to an MLP that predicts whether an edge is active/inactive



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# Obtaining final solutions

- After classifying edges, we get a prediction between 0 and 1 for each edge in the graph.
- We use a simple rounding scheme to obtain the final edge values 0/1 that map to trajectories

 The overall method is reasonably fast (~6 fps) and achieves SOTA in the MOT Challenge by a significant margin

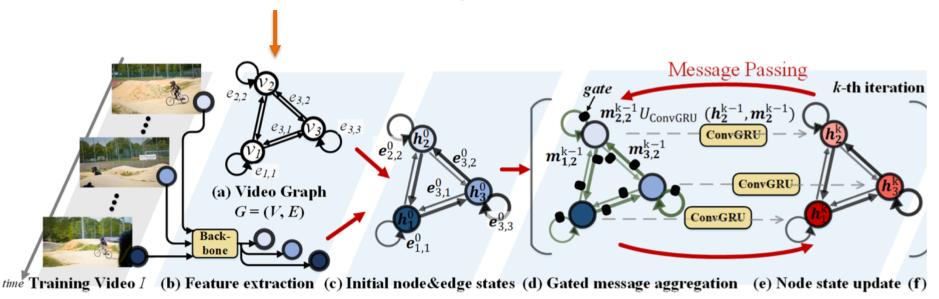
• Goal: Generate accurate and temporally consistent pixel masks for objects in a video sequence.



- Main idea: Model the temporal consistency through a
   Graph Neural Network.
- Each node is a frame, and information is passed among frames to obtain a consistent mask as output

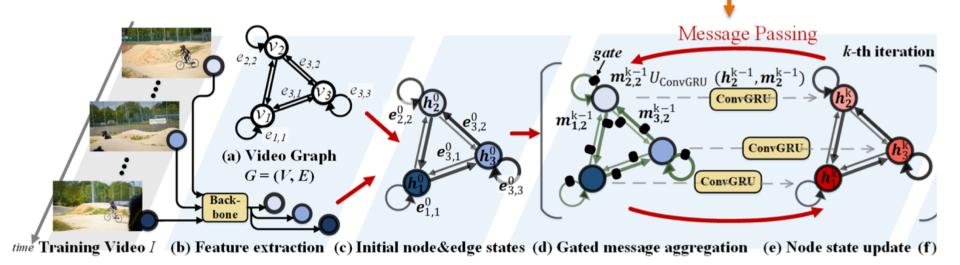
W. Wang et al. "Zero-Shot Video Object Segmentation via Attentive Graph Neural Networks". ICCV 2019.

Features extraction with DeepLabV3 to construct the initial embeddings



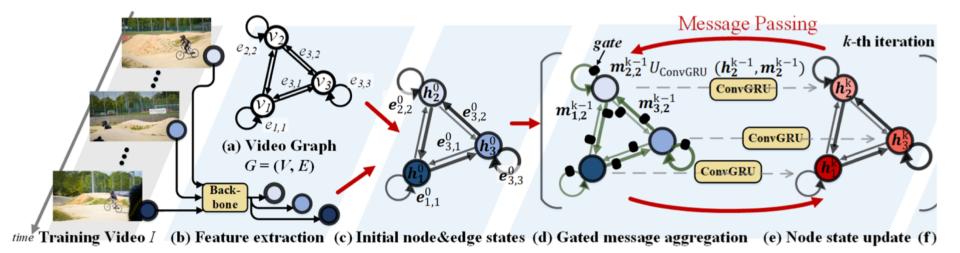
W. Wang et al. "Zero-Shot Video Object Segmentation via Attentive Graph Neural Networks". ICCV 2019.

Message passing with convolutional recurrent networks, since we need to preserve the spatial information (we still want to get pixel outputs)



W. Wang et al. "Zero-Shot Video Object Segmentation via Attentive Graph Neural Networks". ICCV 2019.

• But each pixel is not equally important, so they further propose to use attention  $\rightarrow$  what is that?



W. Wang et al. "Zero-Shot Video Object Segmentation via Attentive Graph Neural Networks". ICCV 2019.

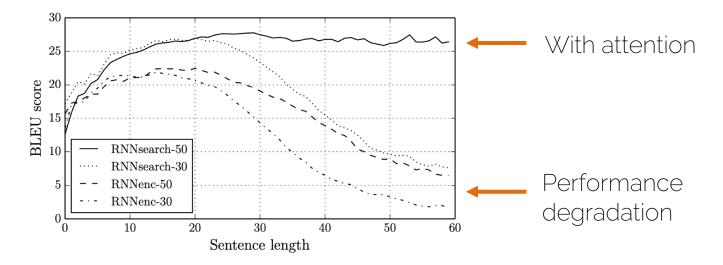


# Attention

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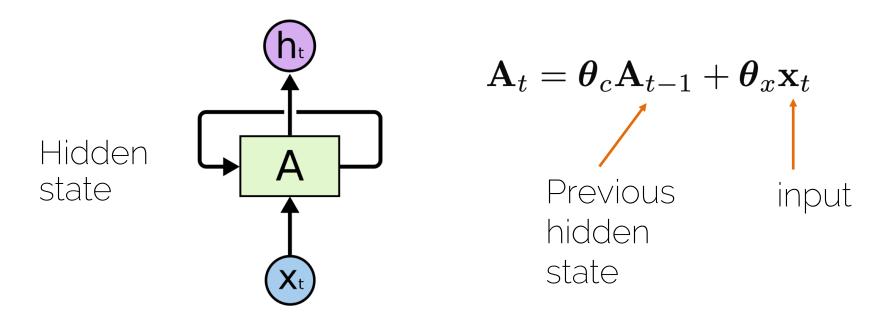
### The problem

• For very long sentences, the score for machine translation really goes down after 30-40 words.

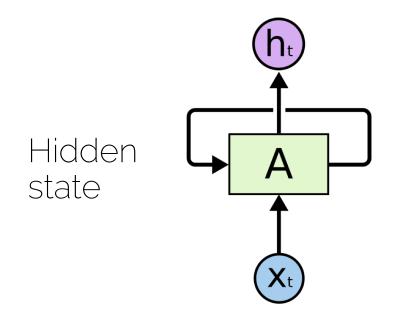


57

• We want to have notion of "time" or "sequence"



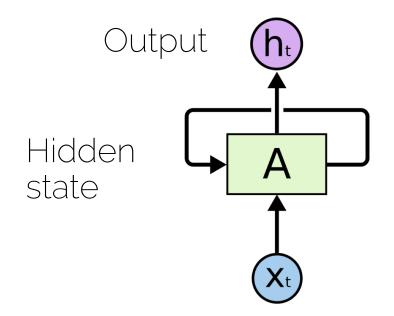
• We want to have notion of "time" or "sequence"



 $\mathbf{A}_t = \boldsymbol{\theta}_c \mathbf{A}_{t-1} + \boldsymbol{\theta}_x \mathbf{x}_t$ 

Parameters to be learned

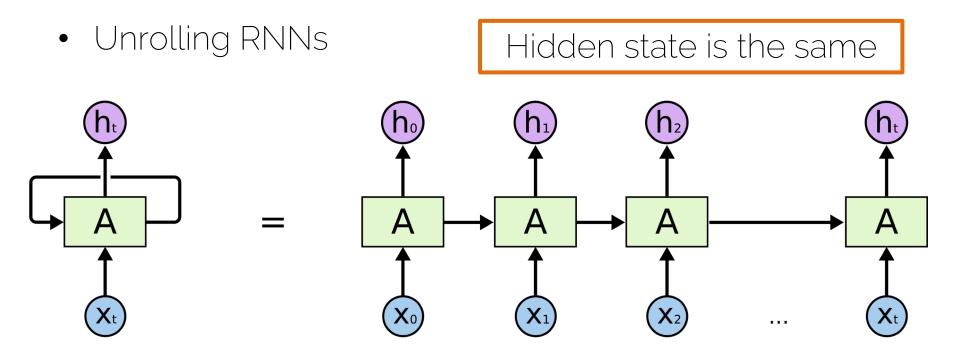
• We want to have notion of "time" or "sequence"



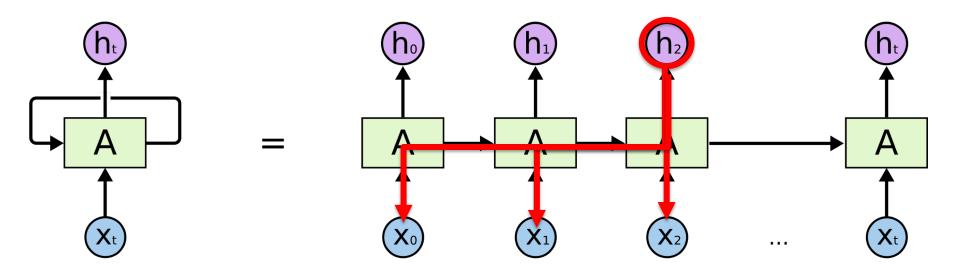
$$\mathbf{A}_t = \boldsymbol{\theta}_c \mathbf{A}_{t-1} + \boldsymbol{\theta}_x \mathbf{x}_t$$

$$\mathbf{h}_t = \boldsymbol{\theta}_h \mathbf{A}_t$$

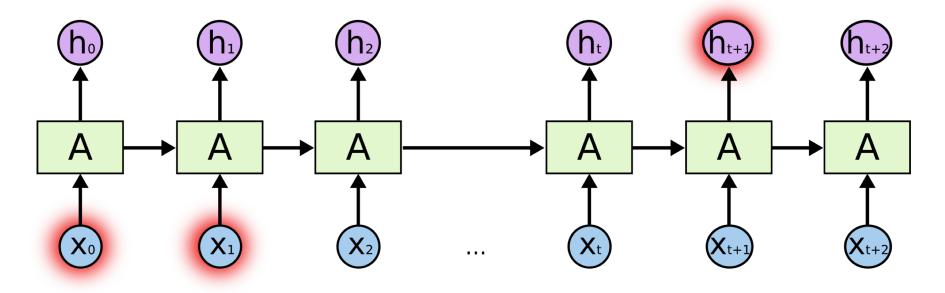
Same parameters for each time step = generalization!



• Unrolling RNNs



#### Long-term dependencies

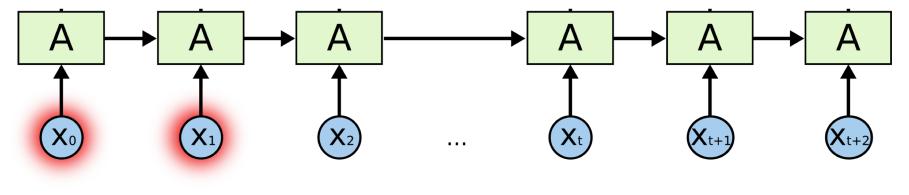


#### I moved to Germany ...

so I speak German fluently

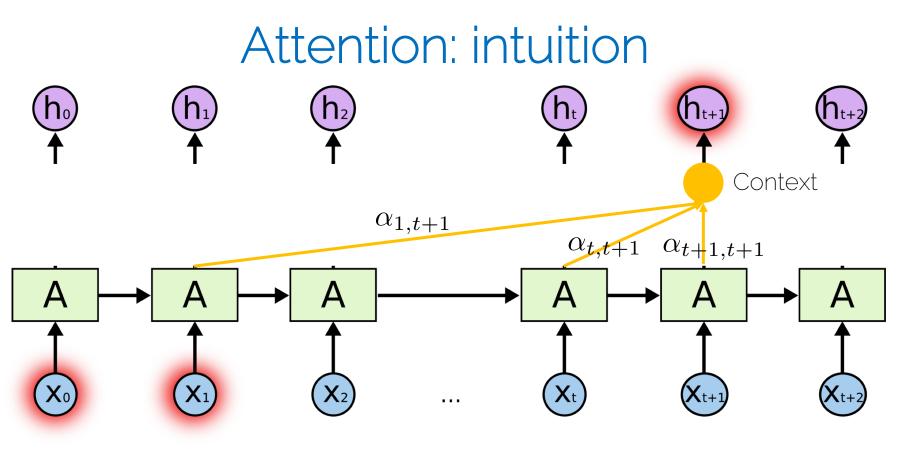


ATTENTION: Which hidden states are more important to predict my output?



#### I moved to Germany ...

so I speak German fluently



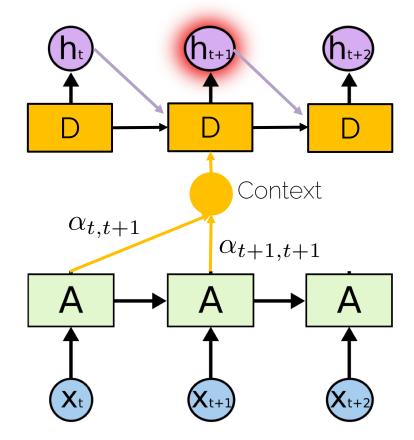
#### I moved to Germany ...

so I speak German fluently

### Attention: architecture

• A decoder processes the information

- Decoders take as input:
  - Previous decoder hidden state
  - Previous output
  - Attention



#### Attention

•  $\alpha_{1,t+1}$  indicates how much the word in the position 1 is important to translate the word in position t+1

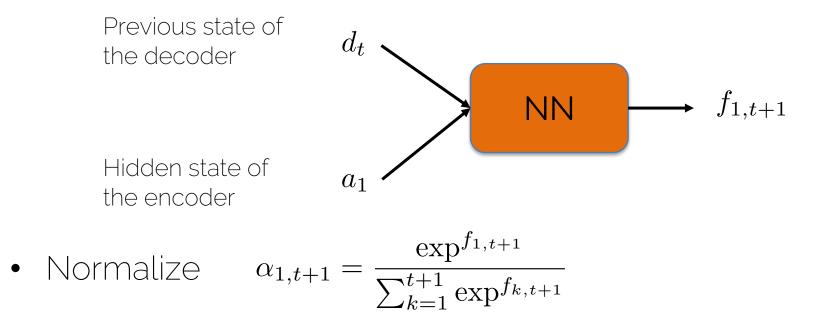
• The context aggregates the attention

$$c_{t+1} = \sum_{k=1}^{t+1} \alpha_{k,t+1} a_k$$

• Soft attention: All attention masks alpha sum up to 1

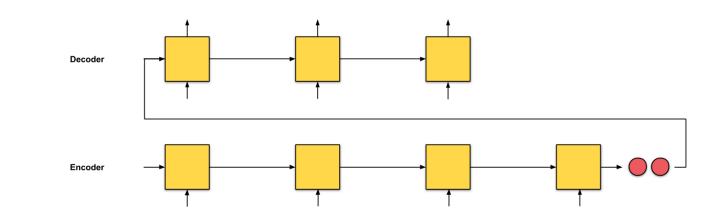
# Computing the attention mask

• We can train a small neural network



Seq2Seq

- How do we translate?
- First read the whole sentence in language 1.
- *Afterwards*, translate the whole sentence in language



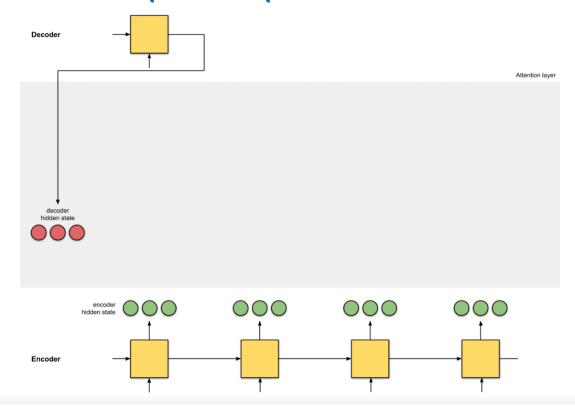
Sutskever et al. "Sequence to Sequence Learning with Neural Networks". NIPS 2014 Picture from: <u>https://towardsdatascience.com/attn-illustrated-attention-5ec4ad276ee3</u>

2.

# Seq2Seq + Attention?

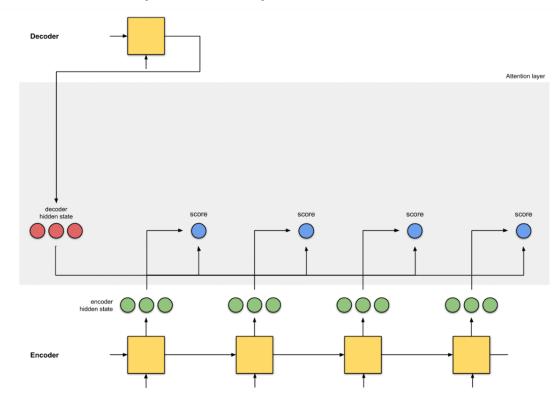
- If the sentence is very long, we might have forgotten what was said at the beginning.
- Solution: take "notes" of keywords as we read the sentence in language 1.
- Use attention!

#### Seq2Seq + Attention

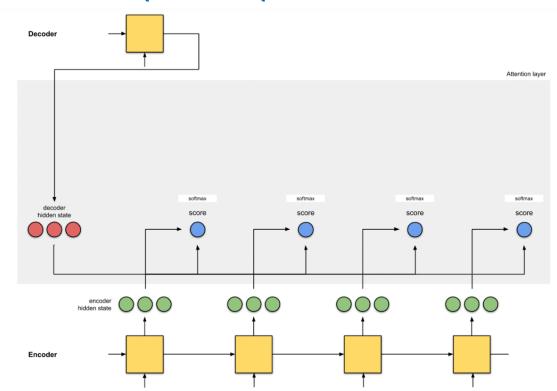


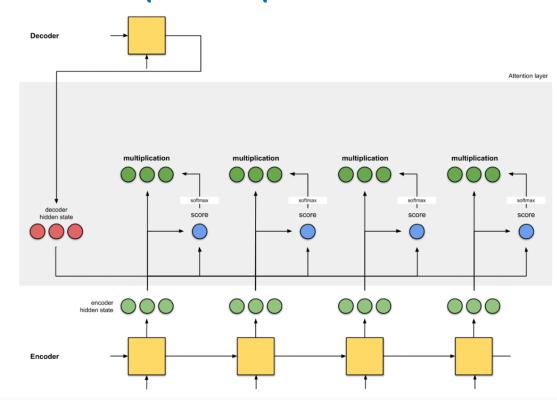
Animation from: https://towardsdatascience.com/attn-illustrated-attention-5ec4ad276ee3

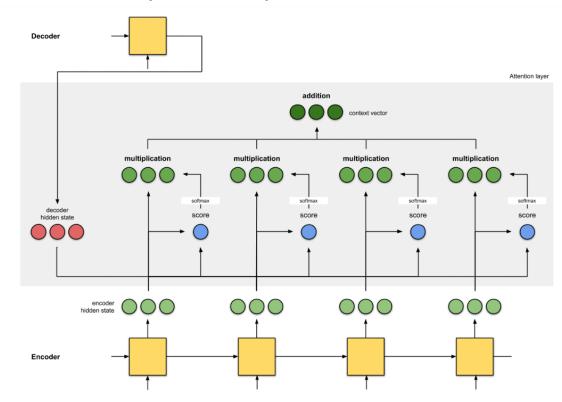
Seq2Seq + Attention

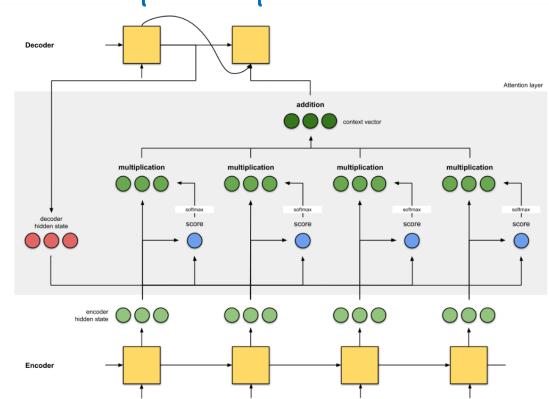


Animation from: https://towardsdatascience.com/attn-illustrated-attention-5ec4ad276ee3



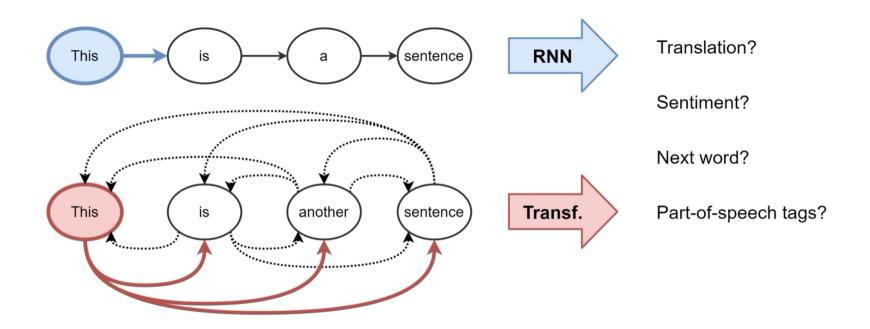




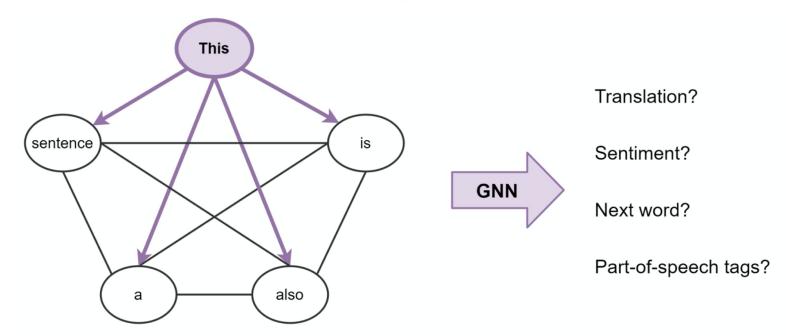


- What if we could get rid of the recurrent architecture and use only attention?
- All the memory problems of RNNs could disappear
- No RNN, no CNN, just attention!

• Current state-of-the-art in NLP!



• Wait, what does this remind you of?



- Broadly speaking, Transformers are based on Graph Attention Networks (GAT)
- GAT replace the aggregation operation of GNN (usually a summation) by a weighted sum, i.e., an attention mechanism

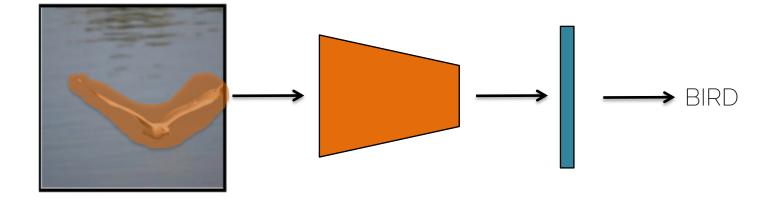


## Attention for vision

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#### Why do we need attention?

• We use the whole image to make the classification



• Are all pixels equally important?

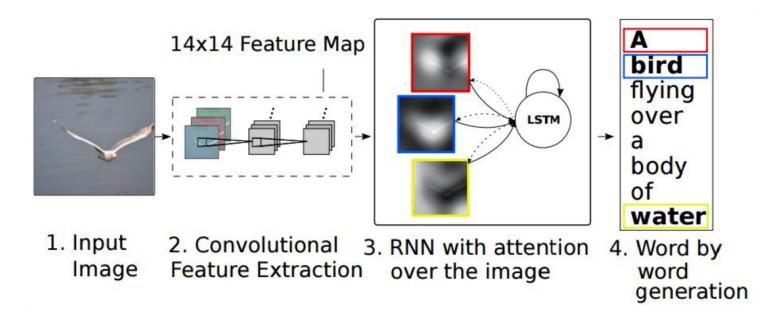
#### Why do we need attention?

• Wouldn't it be easier and computationally more efficient to just run our classification network on the patch?



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#### Image captioning



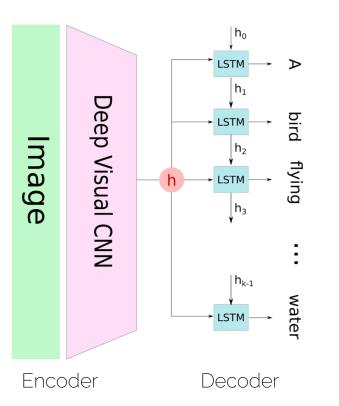
Xu et al 2015. Show attention and tell: neural image caption generation with visual attention.

### Image captioning

- Input: image
- Output: a sentence describing the image.
- Encoder: a classification CNN (VGGNet, AlexNet). This computes a feature maps over the image.
- Decoder: an attention-based RNN
  - In each time step, the decoder computes an attention map over the entire image, effectively deciding which regions to focus on.
  - It receives a context vector, which is the weighted average of the conv net features.

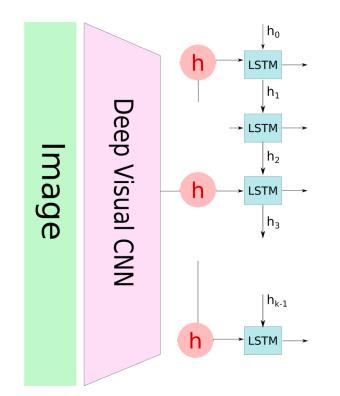
#### **Conventional captioning**





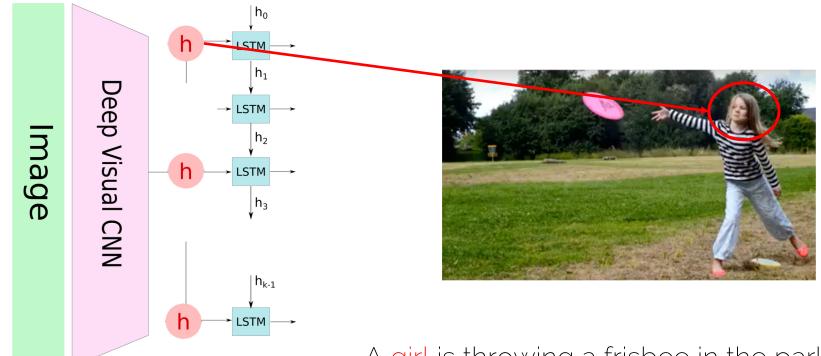
LSTM only sees the image once!

Image from: https://blog.heuritech.com/2016/01/20/attention-mechanism/

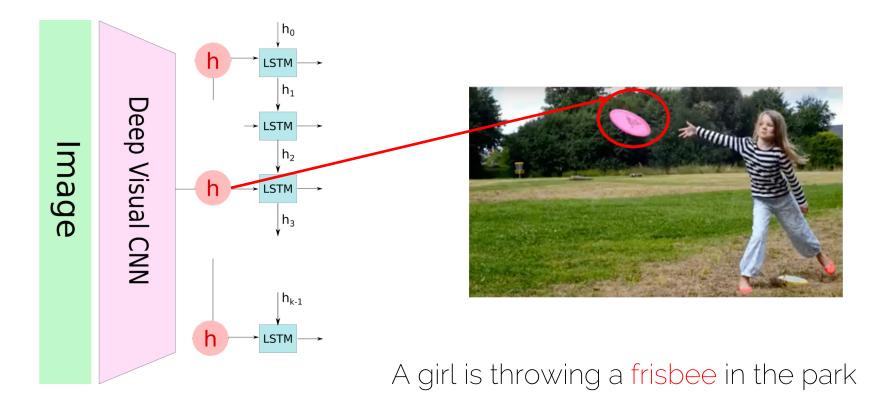


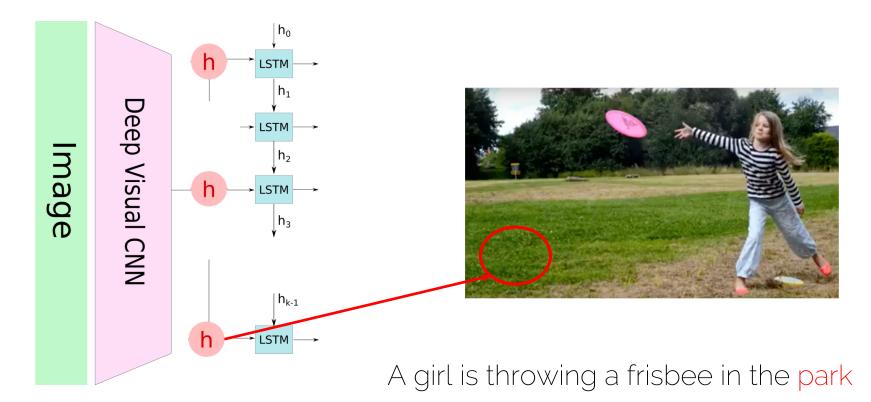


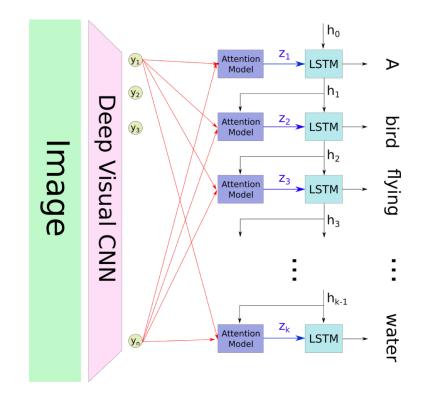
#### A girl is throwing a frisbee in the park



A girl is throwing a frisbee in the park



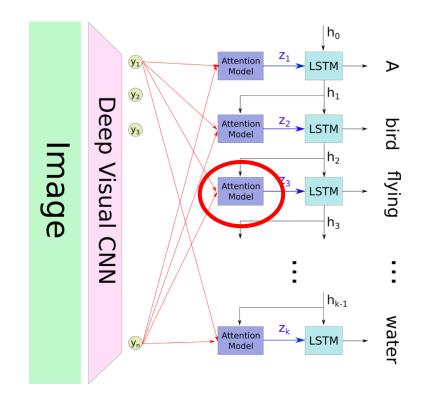




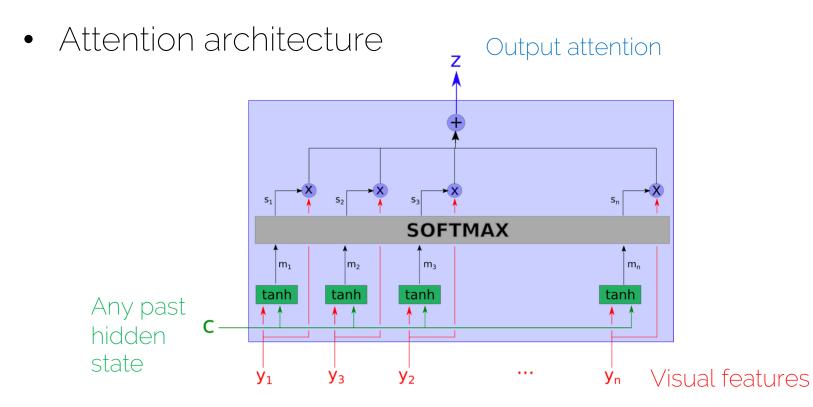
y\_i: Output of encoder are
the image features
which still retain spatial
information (no FC layer!)

Z<sub>i</sub>: Output of attention model

 $h_i$ : Hidden state of LSTM



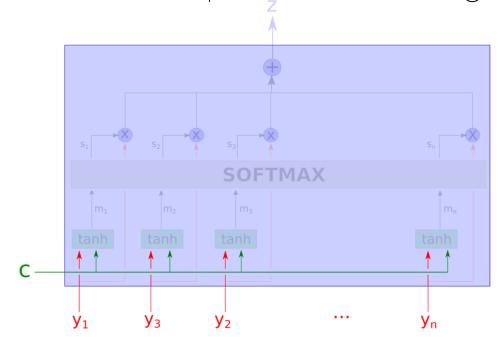
## How does the attention model look like?



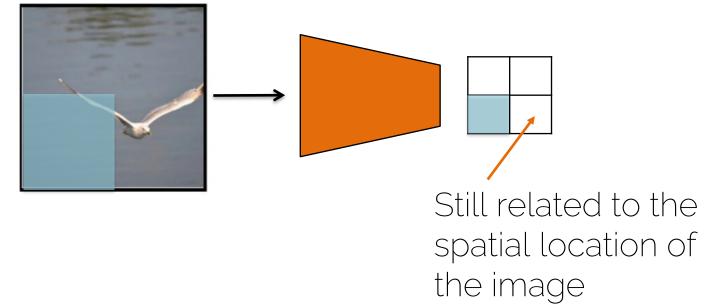
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Image: https://blog.heuritech.com/2016/01/20/attention-mechanism/

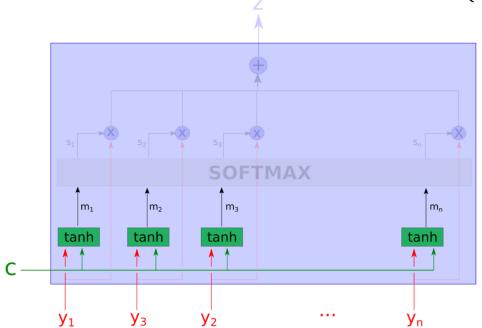
• Inputs = feature descriptor for each image patch



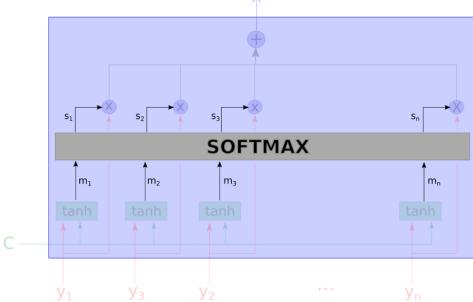
• Inputs = feature descriptor for each image patch



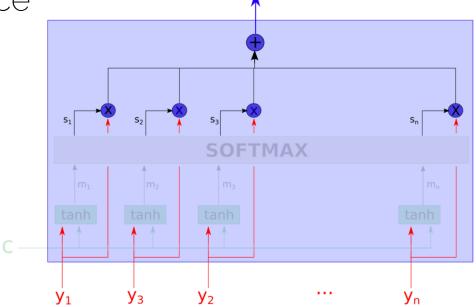
• We want an bounded output  $m_i = \tanh(W_{cm}c + W_{ym}y_i)$ 



 Softmax to create the attention values between 0 and 1

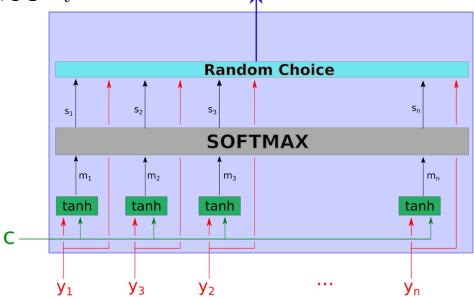


Multiplied by the image features → ranking by importance



#### Hard attention model

• Choosing one of the features by sampling with probabilities  $s_i$ 



#### Types of attention

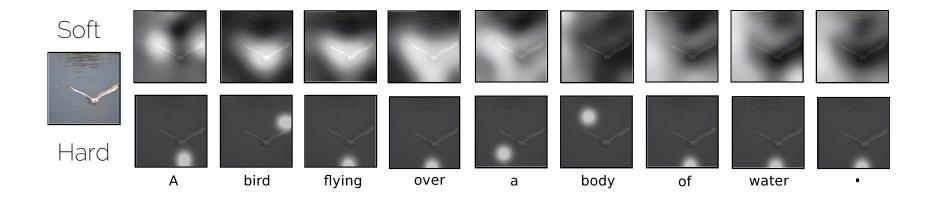
Soft attention: deterministic process that can be backproped

• Hard attention: stochastic process, gradient is estimated through Monte Carlo sampling.

• Soft attention is the most commonly used since it can be incorporated into the optimization more easily

#### Types of attention

• Soft vs hard attention



#### Image captioning with attention



A woman is throwing a frisbee in a park.



A dog is standing on a hardwood floor.



A <u>stop</u> sign is on a road with a mountain in the background.



A little <u>girl</u> sitting on a bed with a teddy bear.



A group of <u>people</u> sitting on a boat in the water.



A giraffe standing in a forest with trees in the background.

Xu et al 2015. Show attention and tell: neural image caption generation with visual attention.



# Deep Learning on graphs

Prof. Leal-Taixé and Prof. Niessner

#### Interesting works on attention

- Luong et al, "Effective Approaches to Attentionbased Neural Machine Translation," EMNLP 2015
- Chan et al, "Listen, Attend, and Spell", arXiv 2015
- Chorowski et al, "Attention-based models for Speech Recognition", NIPS
  2015
- Yao et al, "Describing Videos by Exploiting Temporal Structure", ICCV 2015
- Xu and Saenko, "Ask, Attend and Answer: Exploring Question-Guided Spatial Attention for Visual Question Answering", arXiv 2015
- Zhu et al, "Visual7W: Grounded Question Answering in Images", arXiv 2015
- Chu et al. "Online Multi-Object Tracking Using CNN-based Single Object Tracker with Spatial-Temporal Attention Mechanism". ICCV 2017