Machine Learning: Lecture #3

Jennifer Ngadiuba (Fermilab)
University of Pavia, May 8-12 2023

Overview of the lectures

- **Day 1:**
  - Introduction to Machine Learning fundamentals
  - Linear Models
- **Day 2:**
  - Neural Networks
  - Deep Neural Networks
  - Convolutional Neural Networks
- **Day 3:**
  - Recurrent Neural Networks
  - Graph Neural Networks (part 1)
- **Day 4:**
  - Graph Neural Networks (part 2)
  - Transformers
- **Day 5:**
  - Unsupervised learning
  - Autoencoders
  - Generative Adversarial Networks
  - Normalizing Flows

Hands on sessions each day will closely follow the lectures topics

Lectures are adapted from M. Kagan's courses

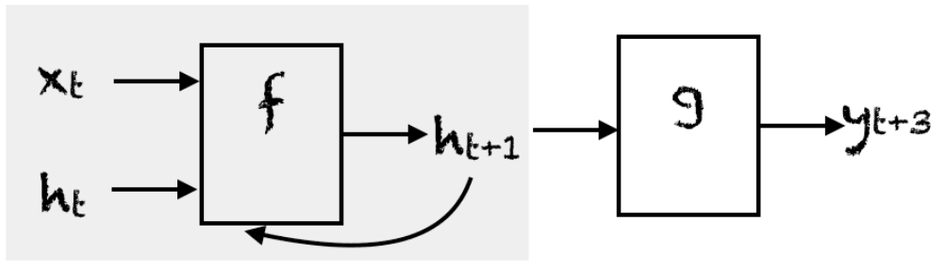
Recurrent Neural Networks

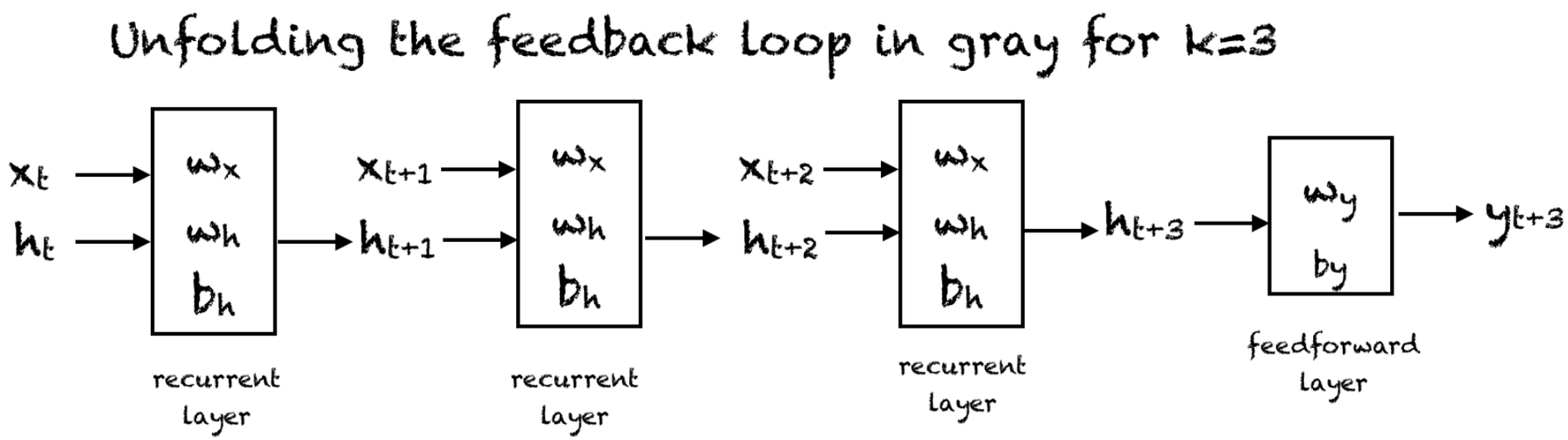
Sequential data

- Many types of data are not fixed in size
- Many types of data have a temporal or sequence-like structure:
  - text
  - video
  - speech
  - DNA
  - …
- MLPs and CNNs expect fixed size data
- How to deal with sequences?

Recurrent Neural Networks

- A **recurrent neural network (RNN)** is a type of NN which processes sequential data
- They are distinguished by their "memory" as they take information from prior inputs to influence the current input and output





Recurrent Neural Networks

- Given a set $\mathcal{X}$, let $S(\mathcal{X})$ be the set of sequences, where each element of the sequence $\mathbf{x}_i \in \mathcal{X}$
  - $\mathcal{X}$ could be reals $\mathbb{R}^m$, integers $\mathbb{Z}^m$, etc…
  - the sequence $x \in S(\mathcal{X})$ has variable length $T(x) \longrightarrow x = \{\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_T\}$
- Use recurrent model that maintains a recurrent state $\mathbf{h}_t \in \mathbb{R}^q$ updated at each time step t:

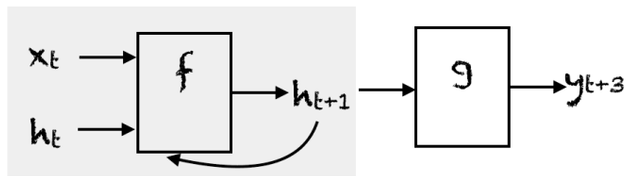
For $t = 1,\ldots,T(x)$: $\quad \mathbf{h}_{t+1} = \phi(\mathbf{x}_t, \mathbf{h}_t; \theta)$

  - simplest model: $\phi(\mathbf{x}_t, \mathbf{h}_t; \mathbf{W}, \mathbf{U}) = \sigma(\mathbf{W}\mathbf{x}_t + \mathbf{U}\mathbf{h}_t)$ ⟶ single MLP with activation σ

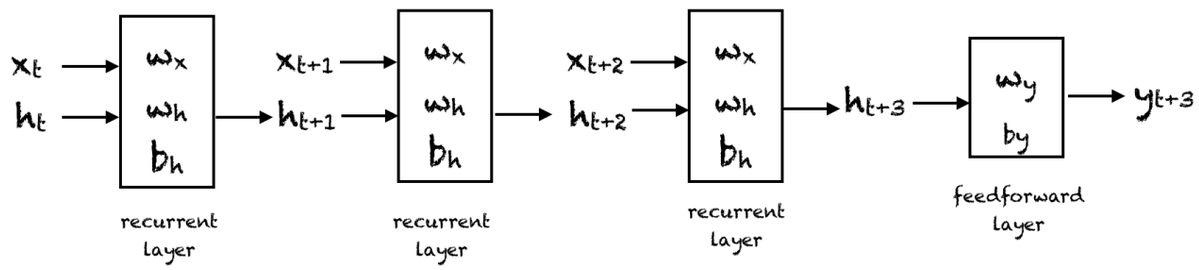
- Predictions can be made at any time step t from the recurrent state:

$$\mathbf{y}_t = \psi(\mathbf{h}_t; \theta)$$

- The hidden state acts as the NN memory — it holds information on previous data the NN has seen



Unfolding the feedback loop in gray for k=3



Recurrent Neural Networks

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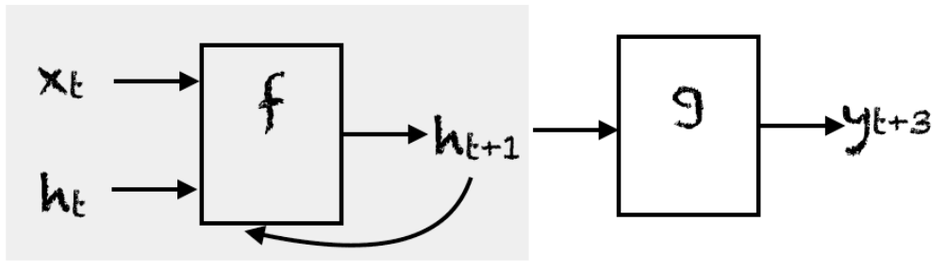
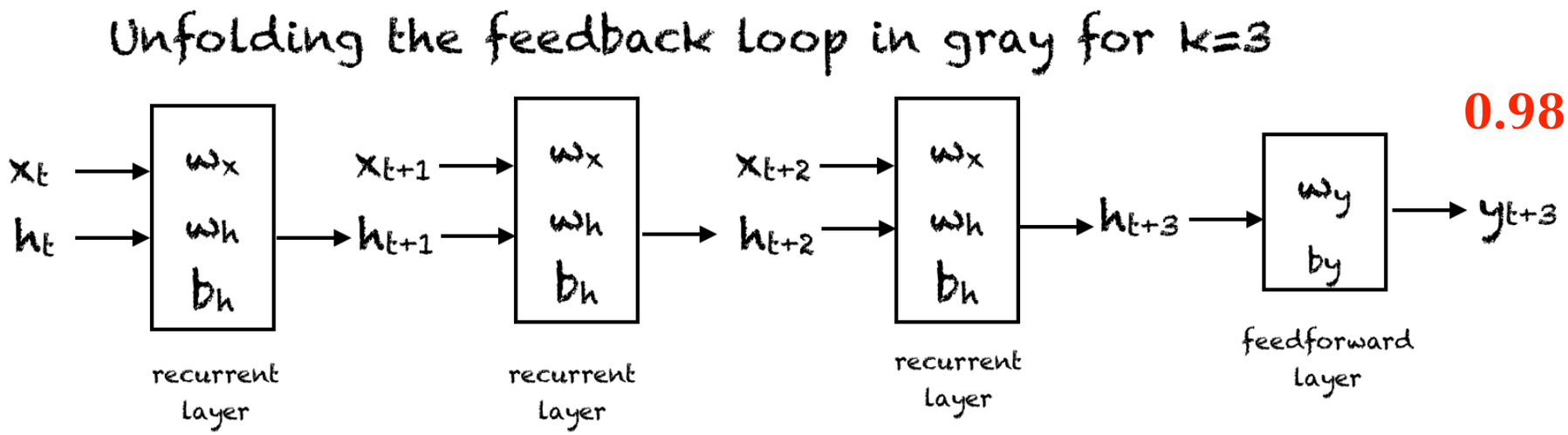


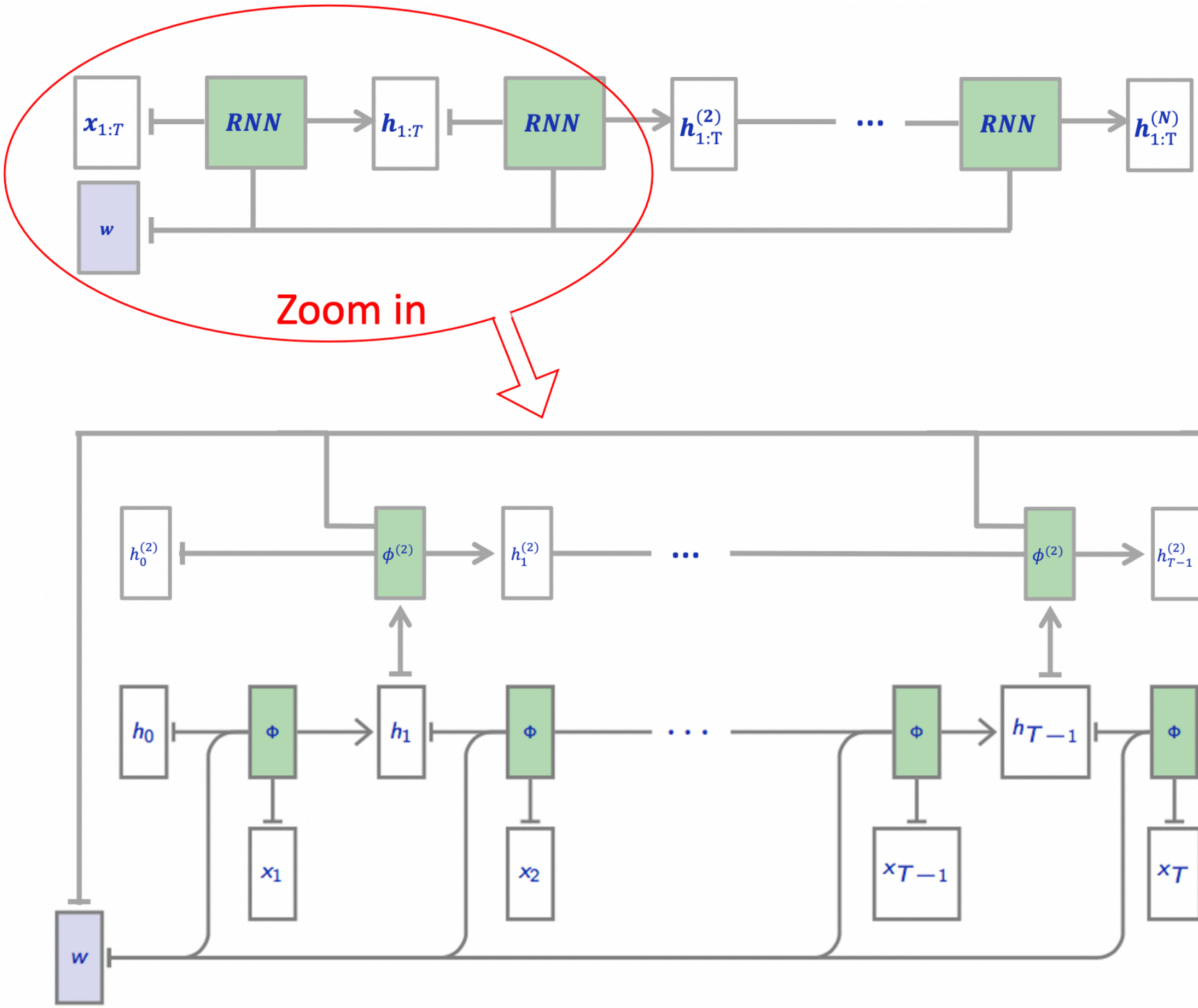


0.98

Positive sentiment

The **movie** **was** **great**

Stacked RNNs



2nd RNN Layer

1st RNN Layer

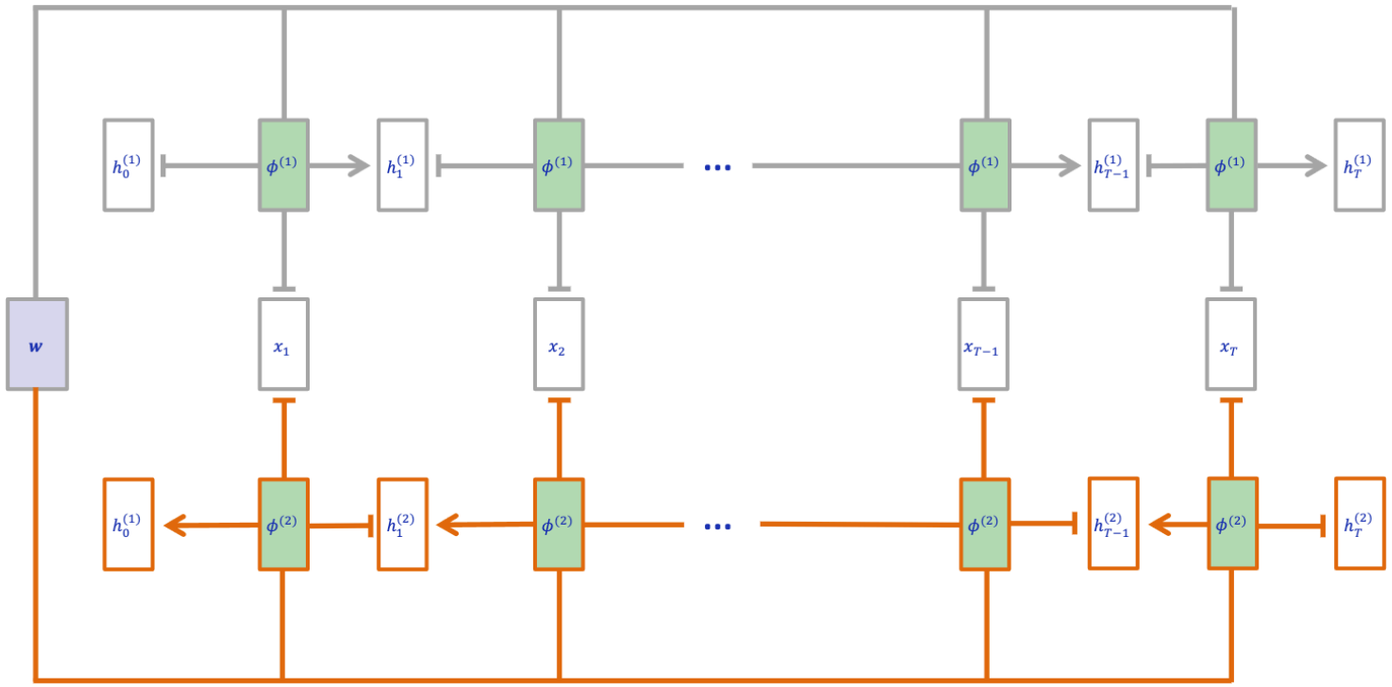
Long Short-Term Memory (LSTM)

- To learn long-term dependency RNNs can grow very big in time → vanishing gradient
  - the layer that get a small gradient update stops and those are typically the earlier layers → short memory

$$\frac{\partial J_n}{\partial W} = \sum_{k=0}^{n} \frac{\partial J_n}{\partial y_n} \frac{\partial y_n}{\partial s_n} \frac{\partial s_n}{\partial s_k} \frac{\partial s_k}{\partial W}$$

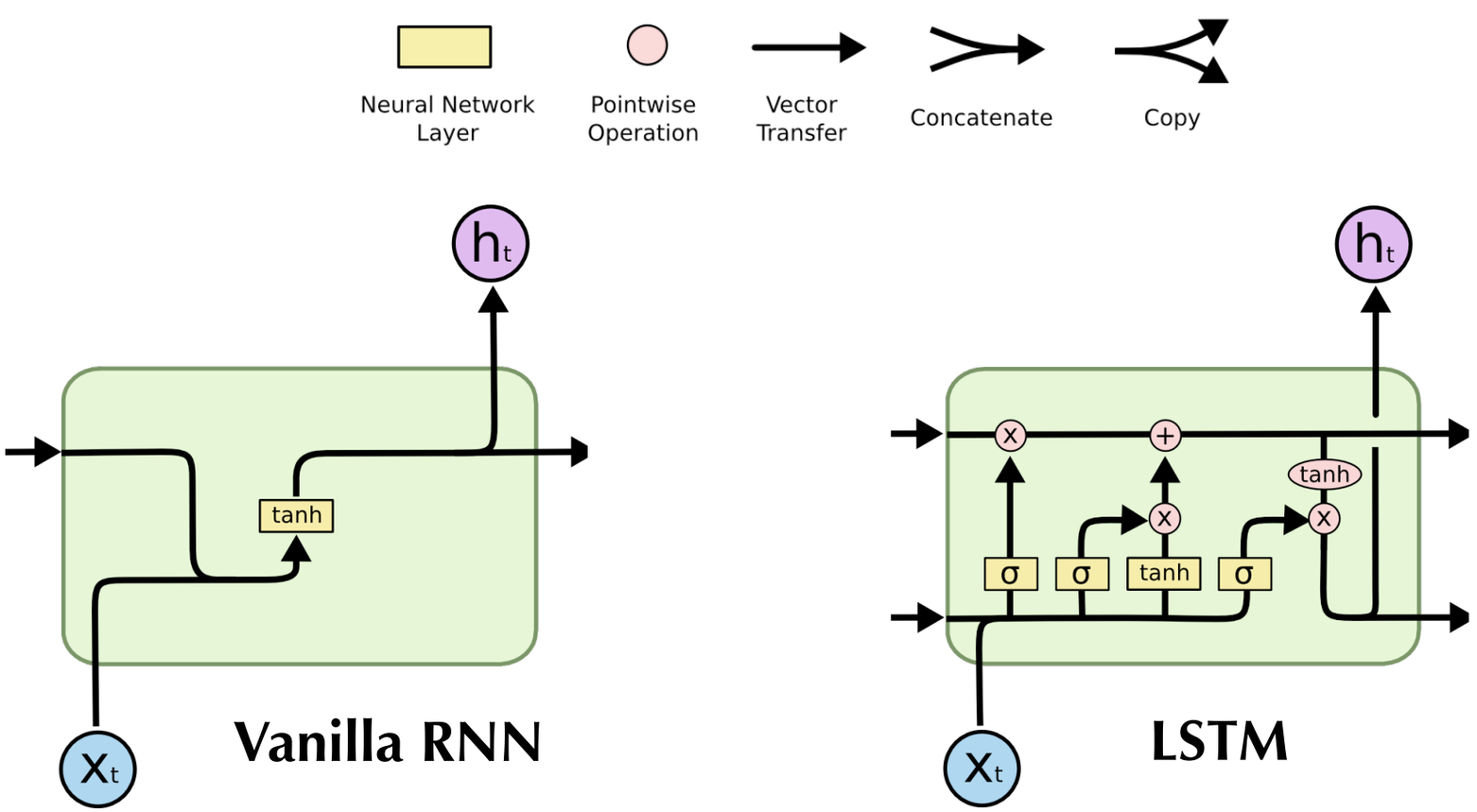
$$\frac{\partial s_n}{\partial s_{n-1}} \frac{\partial s_{n-1}}{\partial s_{n-2}} \cdots \frac{\partial s_3}{\partial s_2} \frac{\partial s_2}{\partial s_1} \frac{\partial s_1}{\partial s_0}$$

[Source]



Long Short-Term Memory (LSTM)

- To learn long-term dependency RNNs can grow very big in time → vanishing gradient
  - the layer that get a small gradient update stops and those are typically the earlier layers → short memory
- Breakthrough from Hochreiter & Schmidhuber (1997) : **Long Short-Term Memory NNs**
  - it can learn to keep only relevant information to make predictions, and forget non relevant data



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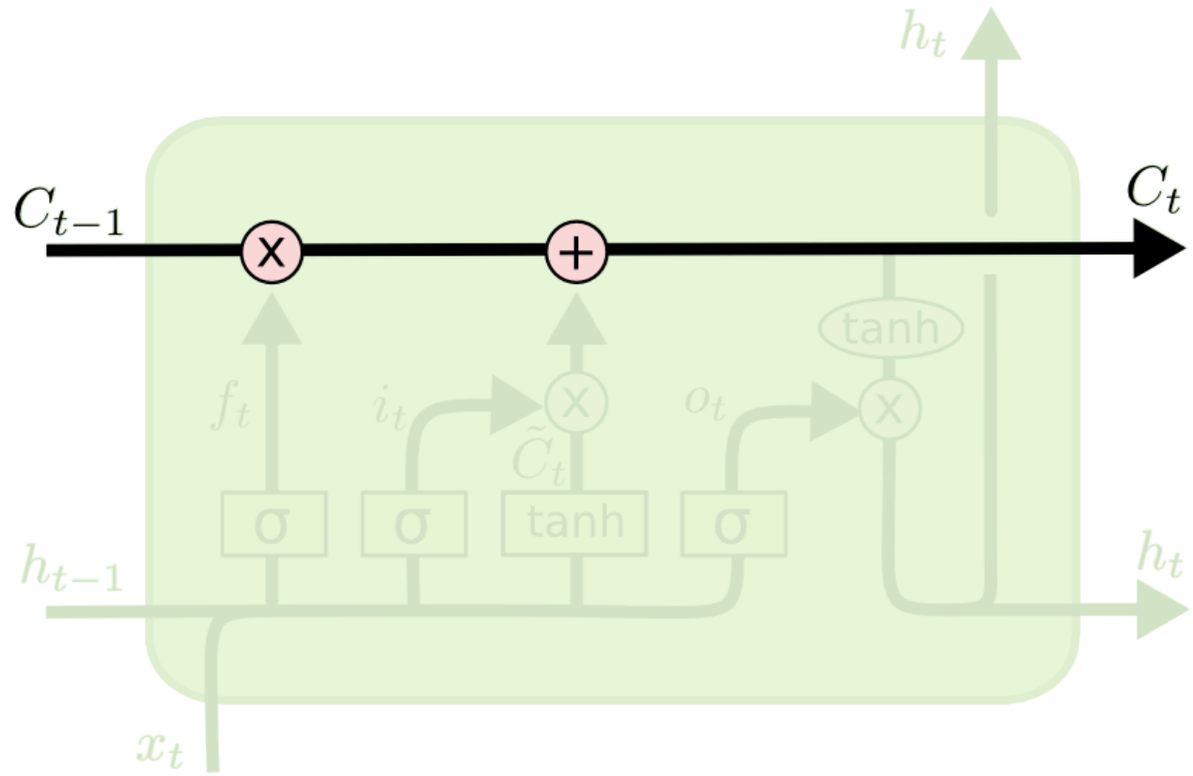
Long Short-Term Memory (LSTM)

- The key to LSTMs is the **cell state** C_t which can thought of as the "long term memory"
  - runs straight down the entire block with only some minor linear interactions
  - allows for information to just flow along it unchanged



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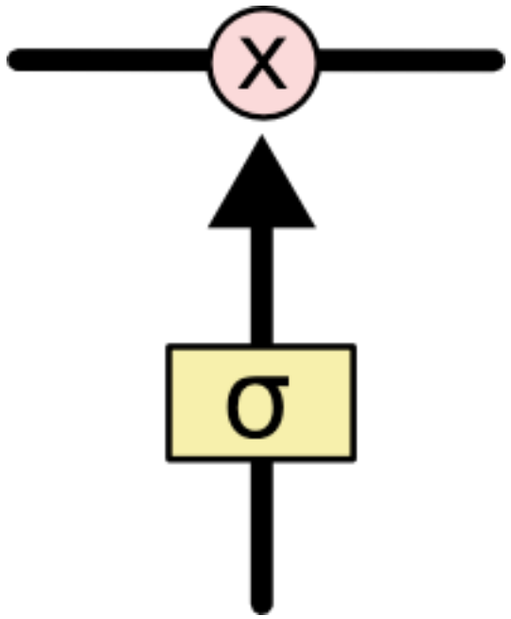
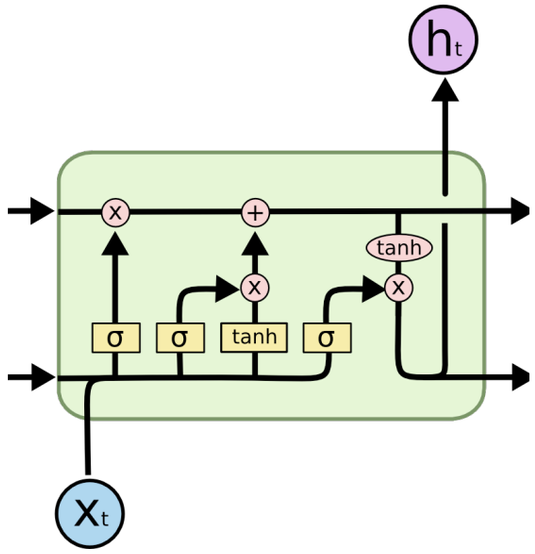
Long Short-Term Memory (LSTM)

- The information that are passed or not to the cell state are controlled by the **gates**
- Gates remove or add information to the cell state through the sigmoid function:
  - a value of zero means “let nothing through”
  - a value of one means “let everything through”
- An LSTM has three of these gates, to protect and control the cell state





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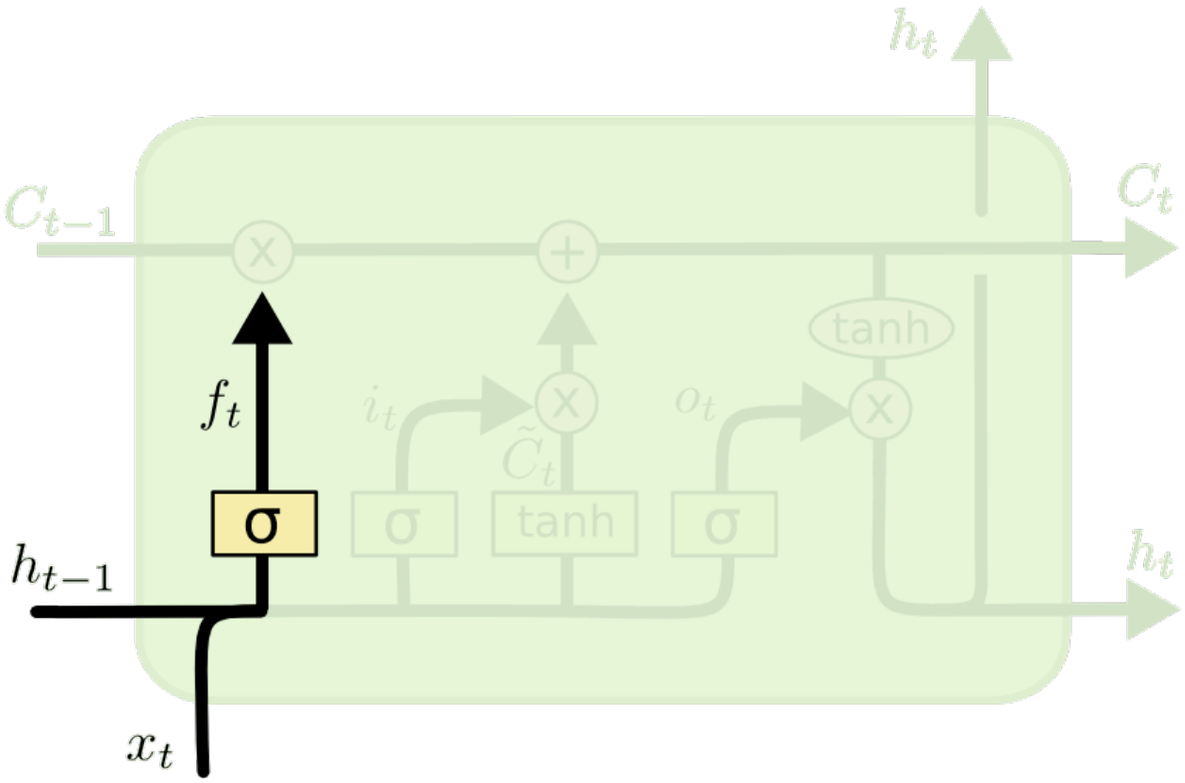
Long Short-Term Memory (LSTM)

- **Forget gate layer:** decide how much of the past information the cell state should forget



$$f_t = \sigma\left(W_f \cdot [h_{t-1}, x_t] \; + \; b_f\right)$$

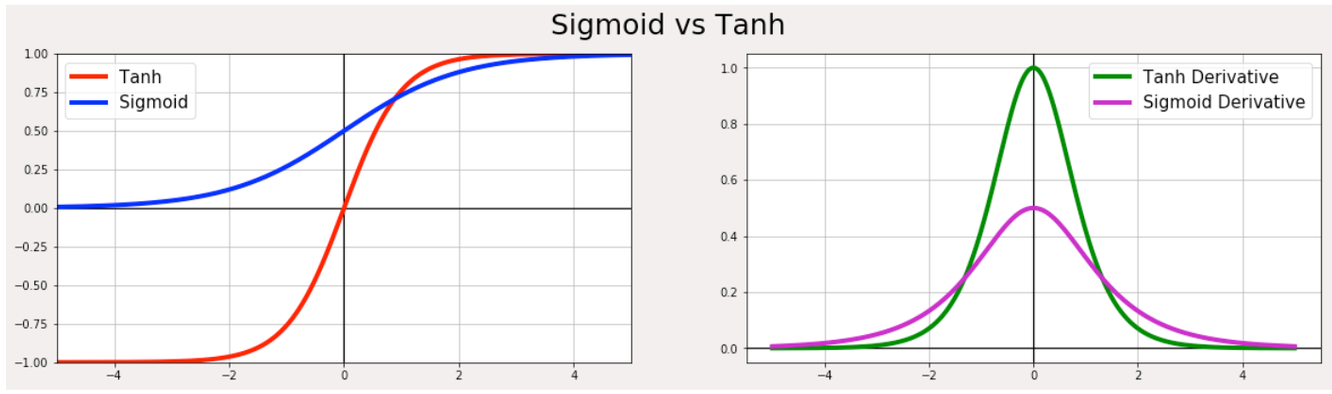
[Source]

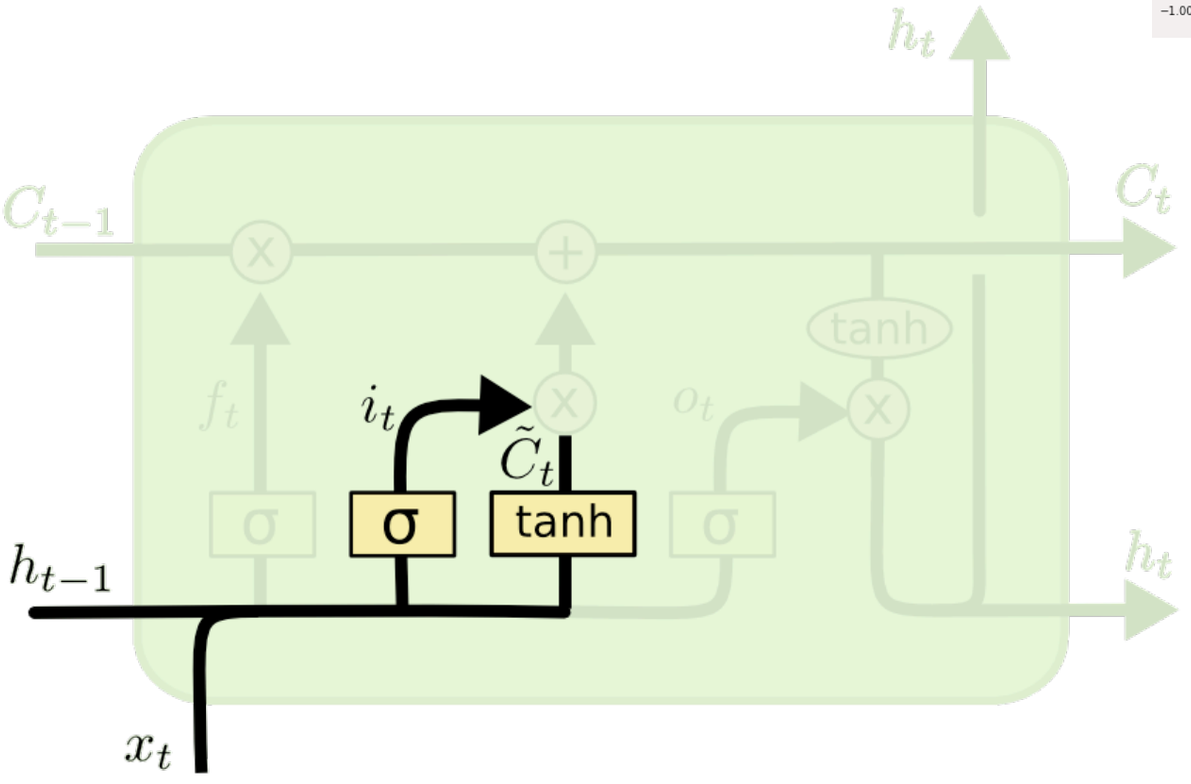
Long Short-Term Memory (LSTM)

- The next step is to decide what new information we are going to store in the cell state

1. the **input gate layer** decides which new values of the current memory are important (through sigmoid)

2. a **tanh layer** allows for negative values to be able to reduce the impact of a component in the cell state — also acts as regularizer



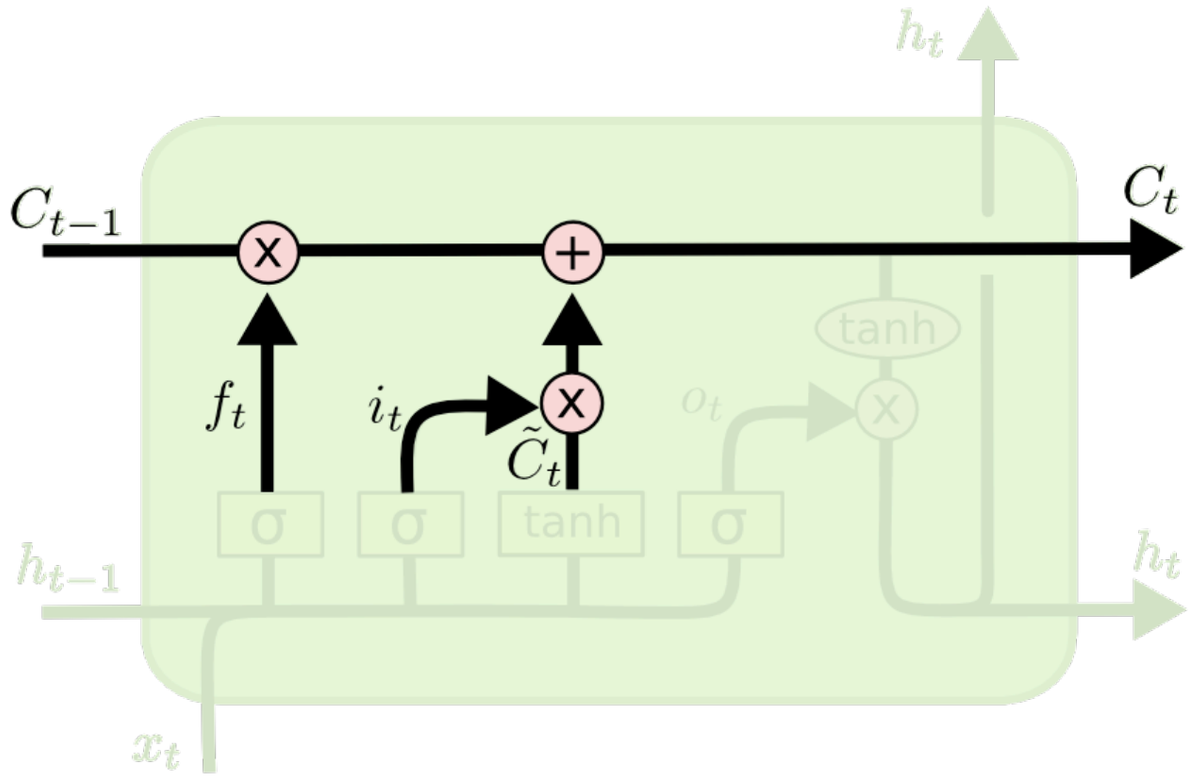


$$i_t = \sigma\left(W_i \cdot [h_{t-1}, x_t] \; + \; b_i\right)$$

$$\tilde{C}_t = \tanh(W_C \cdot [h_{t-1}, x_t] \; + \; b_C)$$

Long Short-Term Memory (LSTM)

- Now we want to update the old cell state C_{t-1} into the new cell state C_t
  - the previous steps already decided what to do, we just need to actually do it.
- We multiply the old state by f_t — which has forgotten the things we decided to forget earlier
- Then we add $i_t \times \tilde{C}_t$ — this is the new memory update vector (as in standard RNN), scaled by how much we decided to update each state value



$$C_t = f_t * C_{t-1} + i_t * \tilde{C}_t$$

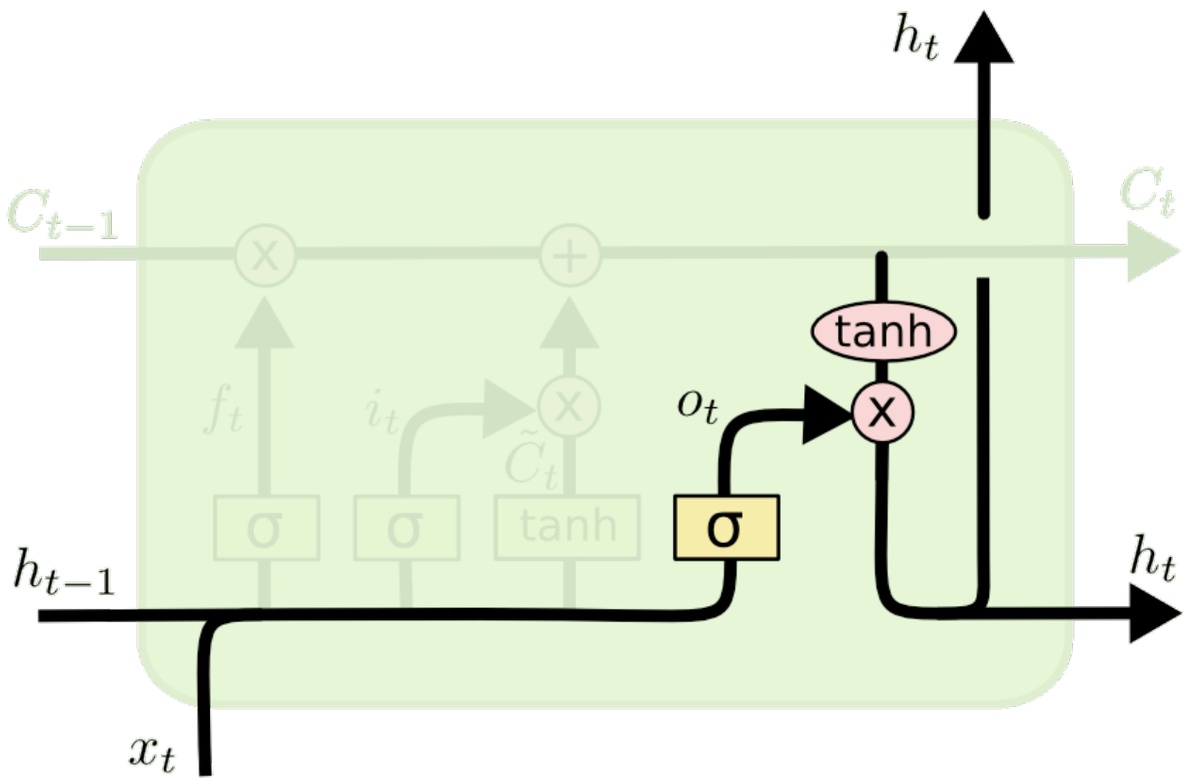
[Source]

Long Short-Term Memory (LSTM)

- Finally, we need to decide what we are going to expose to the next recurrent unit — the output must be based on the current updated cell state

  - an **output gate** decides what part of current memory should be saved to the new hidden state

  - put the current cell state through *tanh* and multiply it by the output of the sigmoid gate, so that we only output the parts we decided to

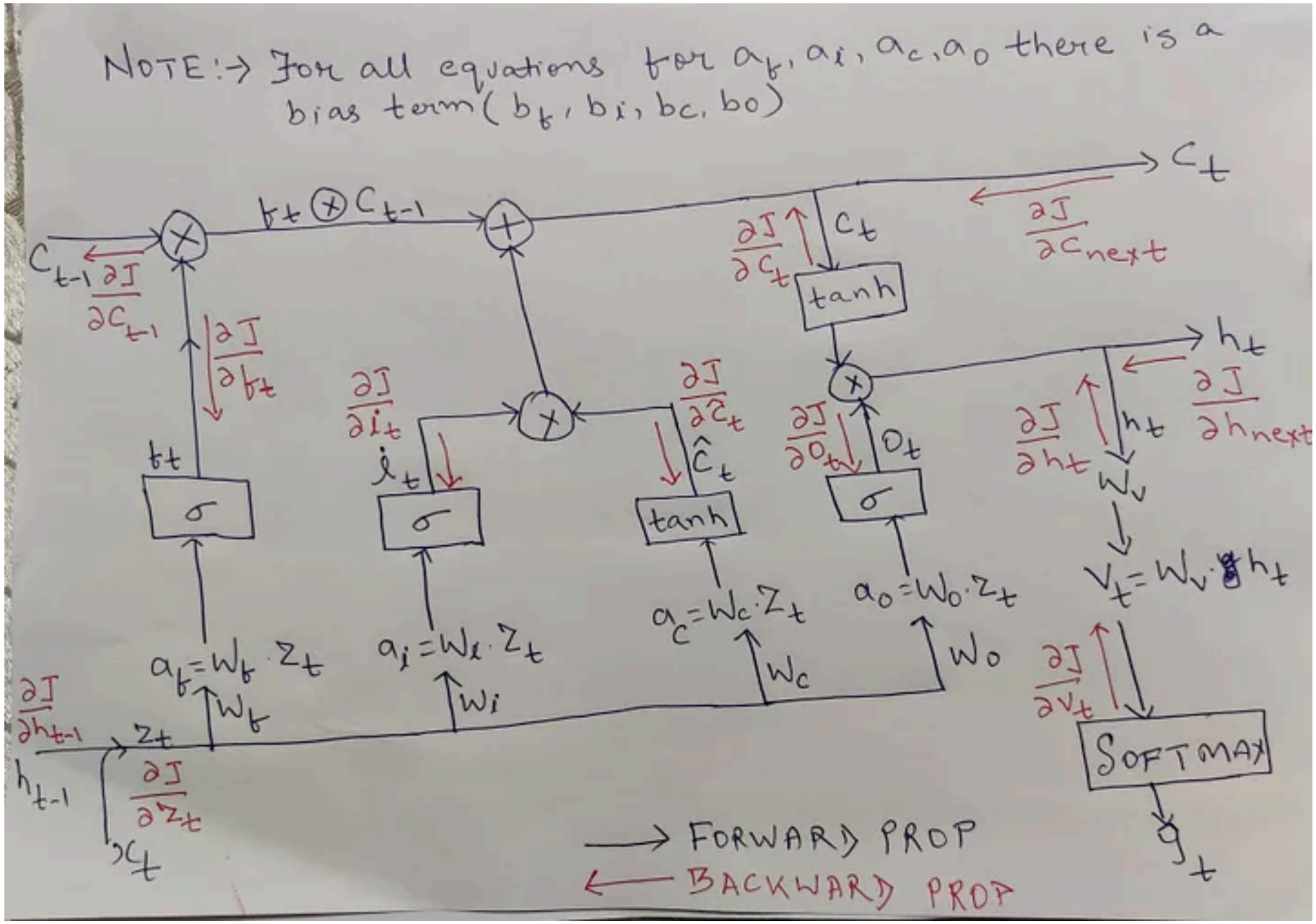


$$o_t = \sigma\left(W_o\ [h_{t-1}, x_t]\ +\ b_o\right)$$

$$h_t = o_t * \tanh\left(C_t\right)$$

[Source]

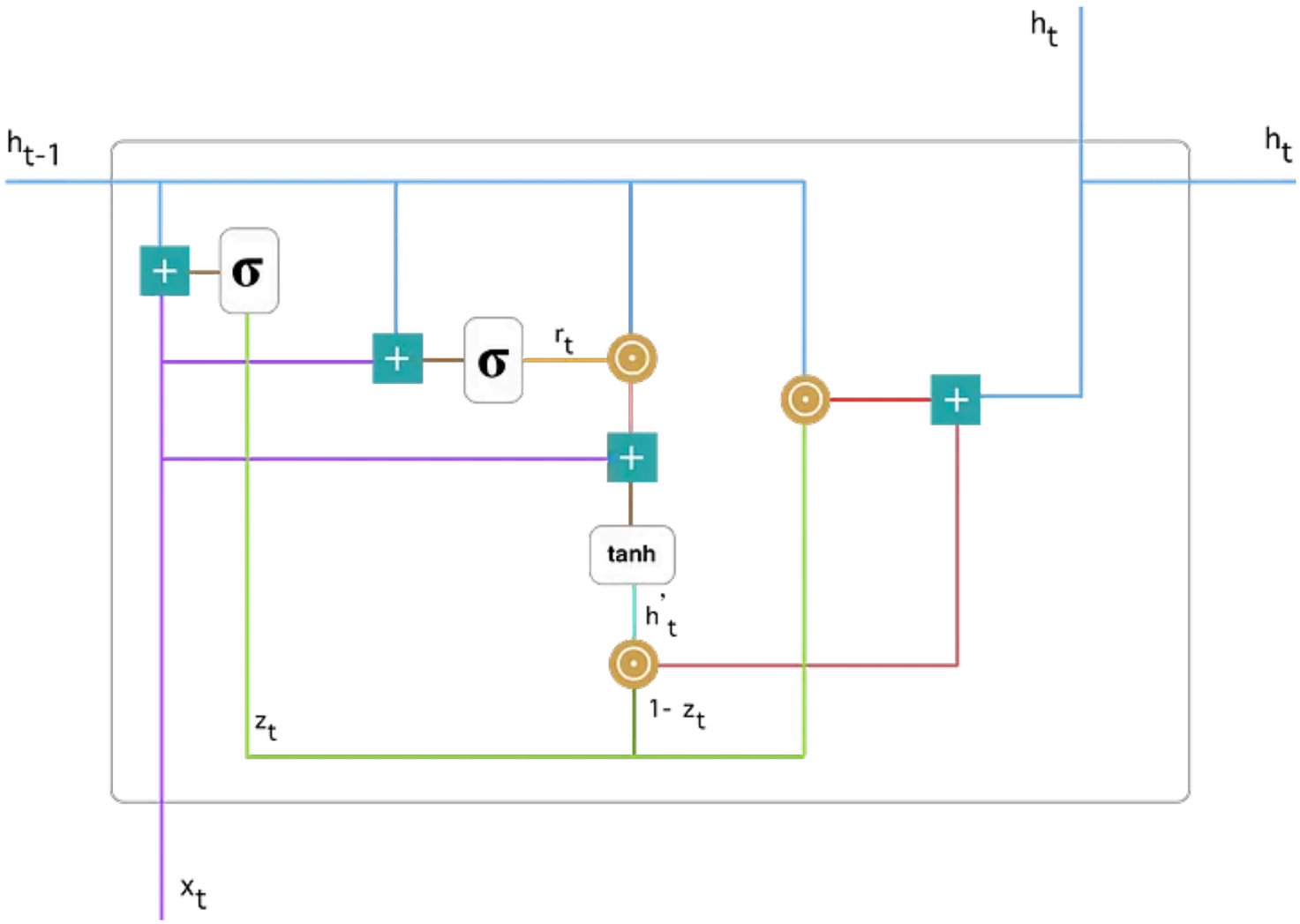
Why do LSTM solve the vanishing gradient problem?



https://towardsdatascience.com/lstm-gradients-b3996e6a0296

Gated Recurrent Unit (GRU)

- GRUs are another variant of RNNs that solve the vanishing gradient problem
  - younger than LSTM — introduced in 2014 by Kyunghyun Cho et al.
  - more computationally efficient than LSTM (2 gates instead of 3) but lower accuracy



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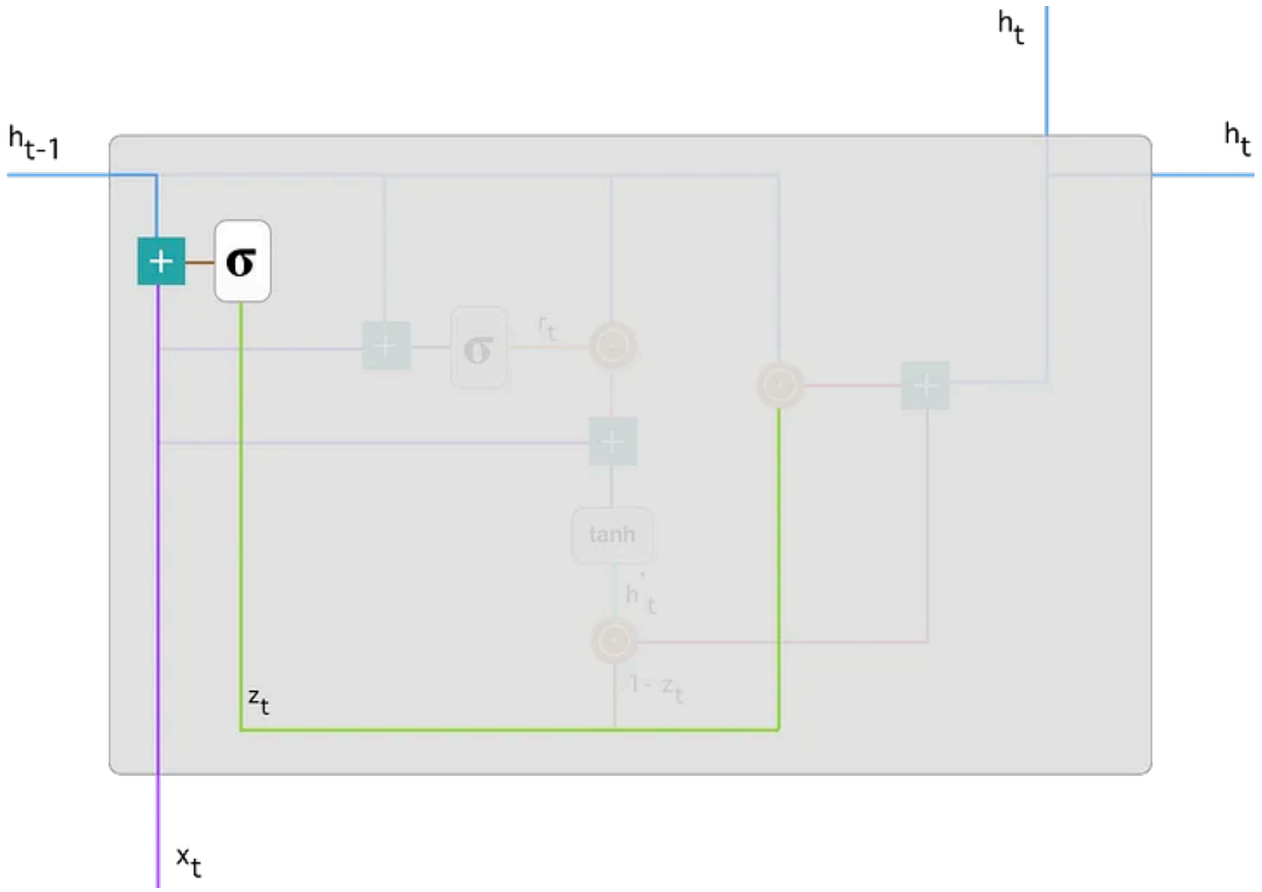
Gated Recurrent Unit (GRU)

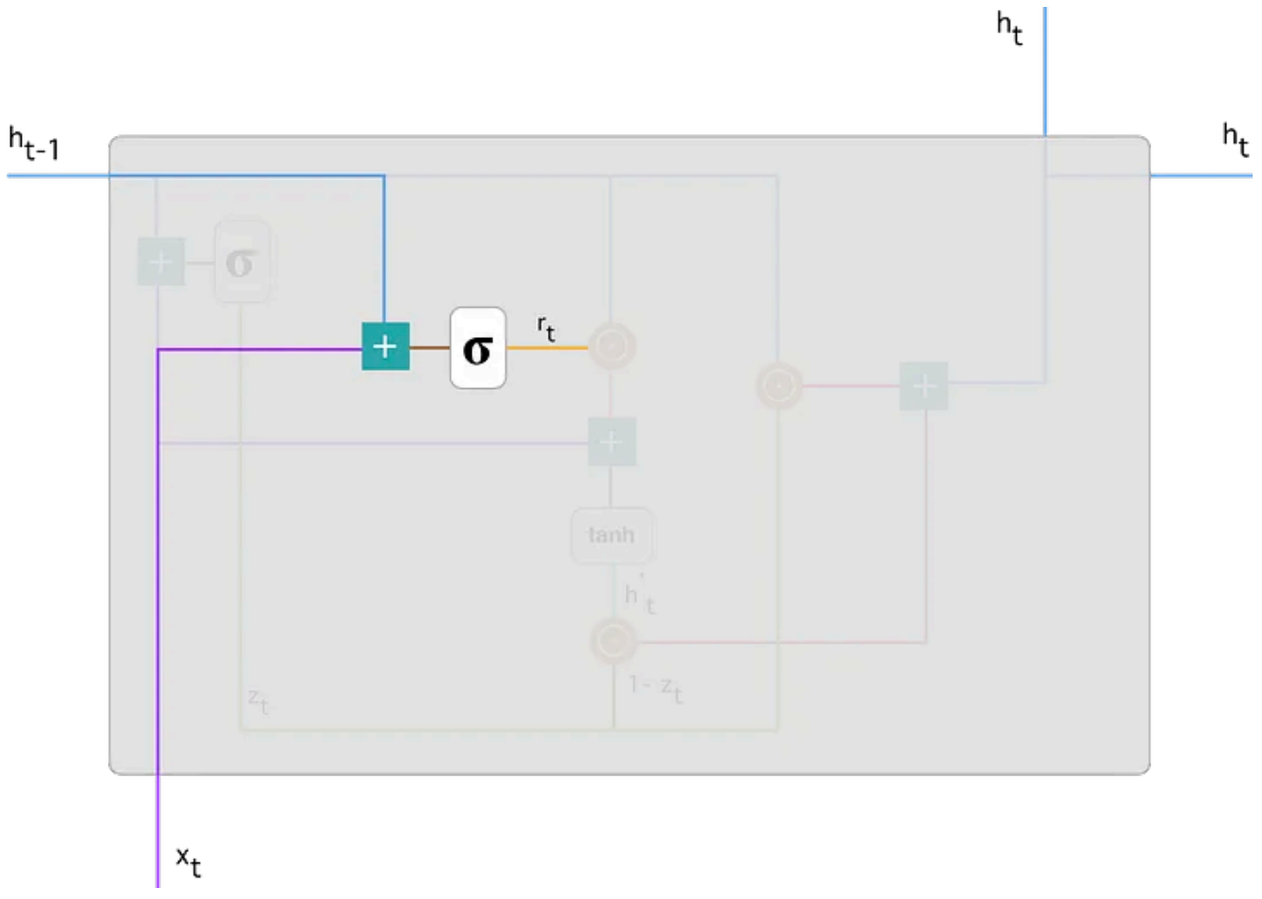
- **Update gate** controls how much of the past information (from previous time steps) needs to be passed along to the future (~ LSTM input gate)



$$z_t = \sigma(W^{(z)}x_t + U^{(z)}h_{t-1})$$

Gated Recurrent Unit (GRU)

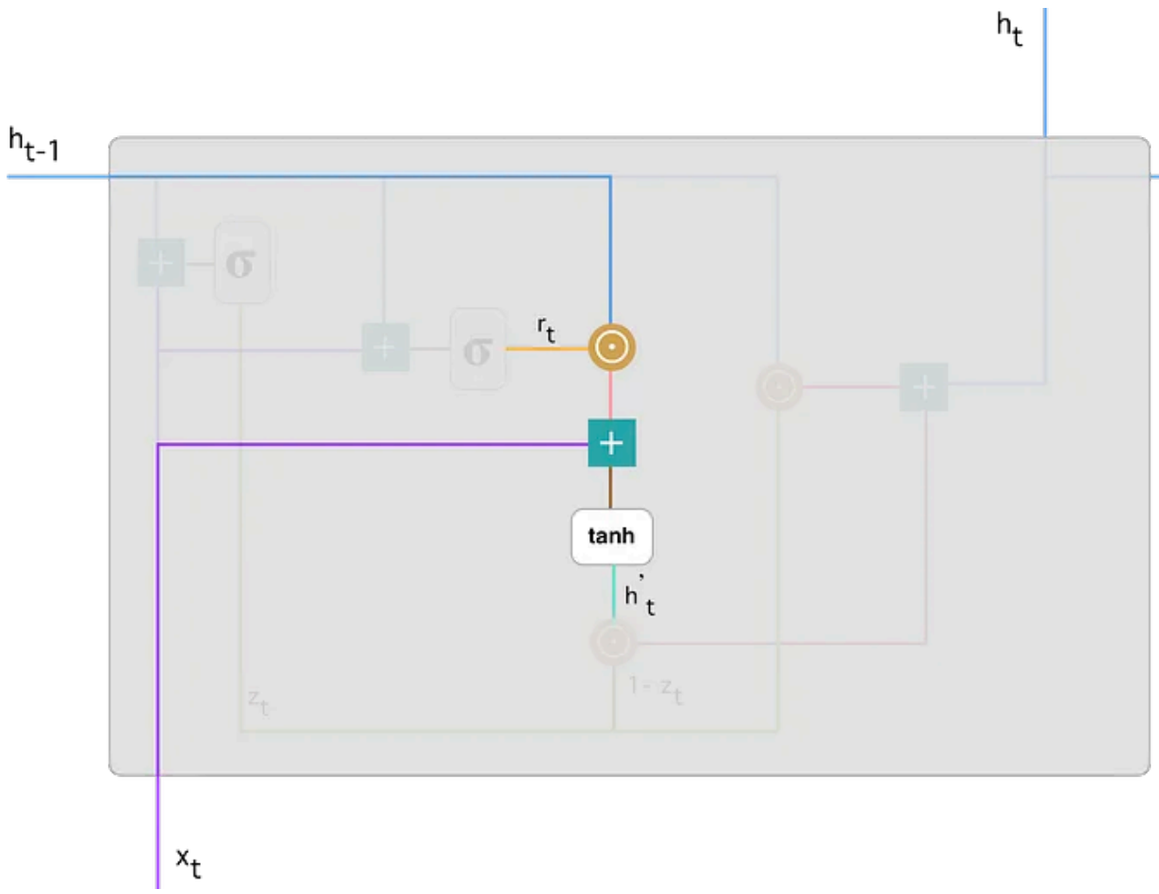
- **Reset gate** is used from the model to decide how much of the past information to forget (~ LSTM forget gate)



$$r_t = \sigma(W^{(r)}x_t + U^{(r)}h_{t-1})$$

Gated Recurrent Unit (GRU)

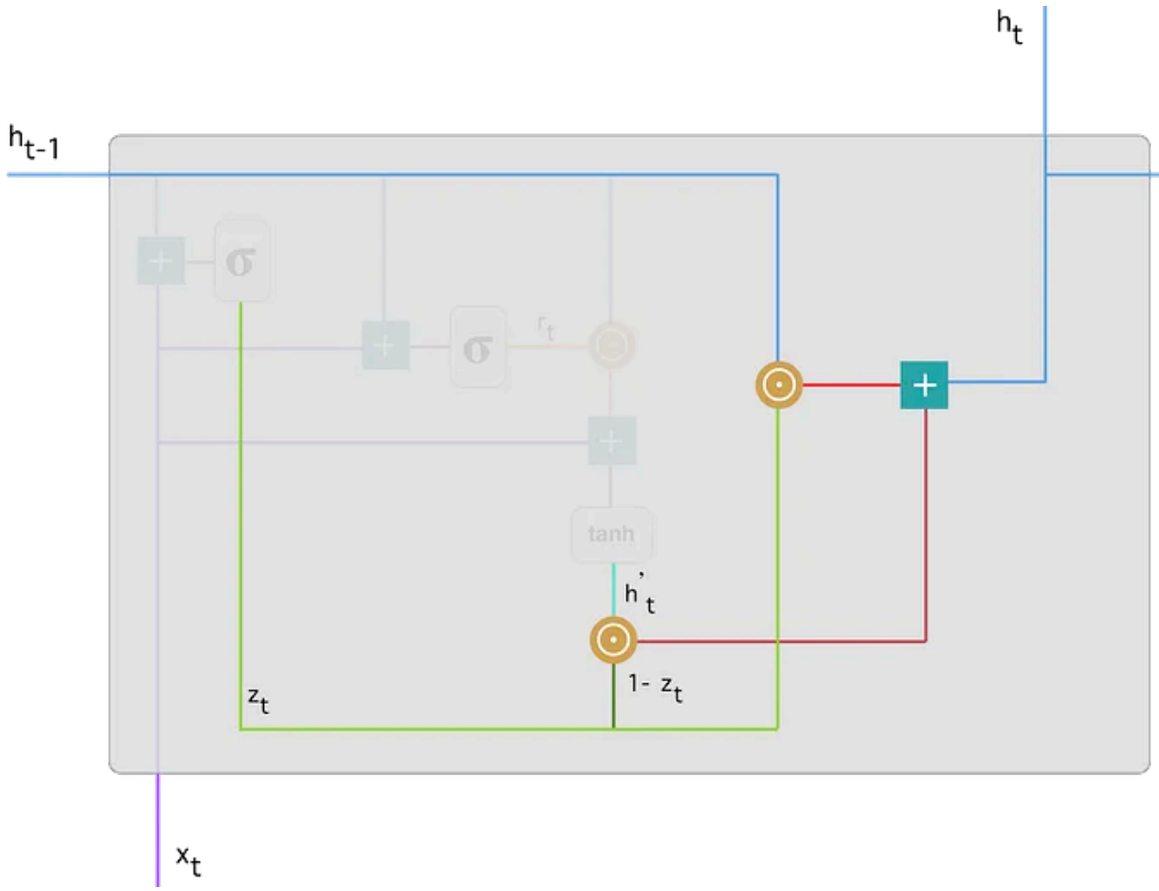
- The **current unit memory content** h_t' is created using the reset gate to store the relevant information from the past



$$h_t' = \tanh(Wx_t + r_t \odot Uh_{t-1})$$

Gated Recurrent Unit (GRU)

- The **new hidden state** h_t — the vector which holds information for the current unit and passes it down to the network — is computed with the update gate

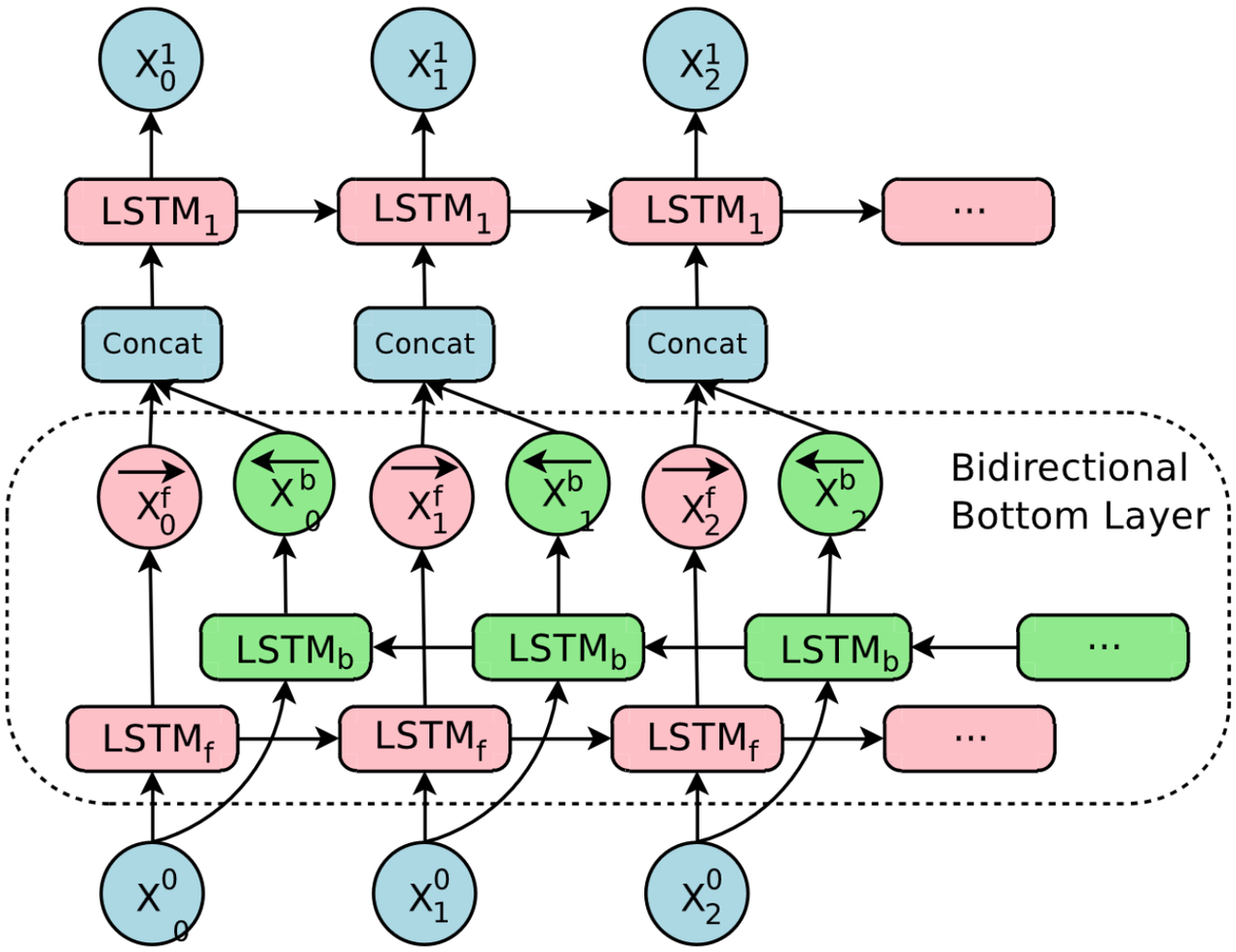


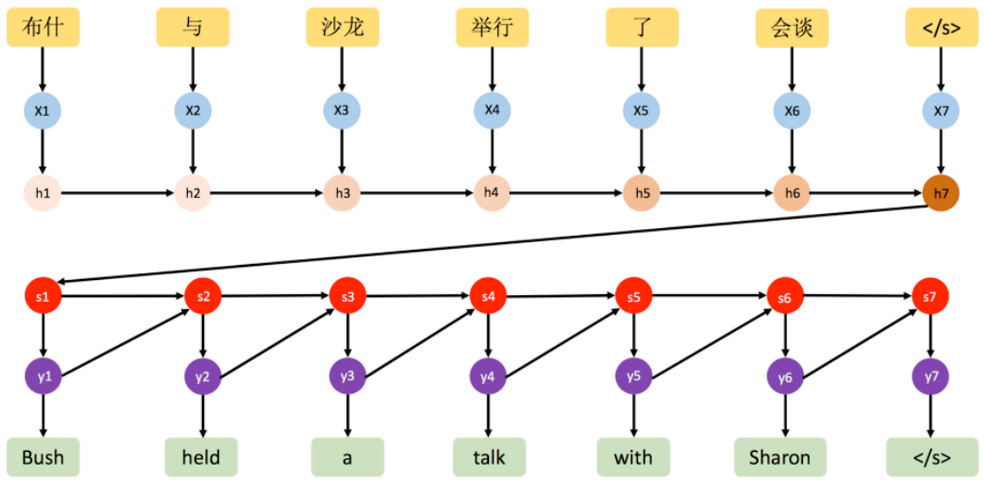
$$h_t = z_t \odot h_{t-1} + (1 - z_t) \odot h'_t$$

Applications of RNNs

Neural Machine Translation

ex, Google Translate model





(Sutskever et al., 2014)

[Y. Wu et al., 2016]

Applications of RNNs

Speech Recognition

ex, Alexa or Siri

The other way around is text-to-speech:
see Shen et al, 2017

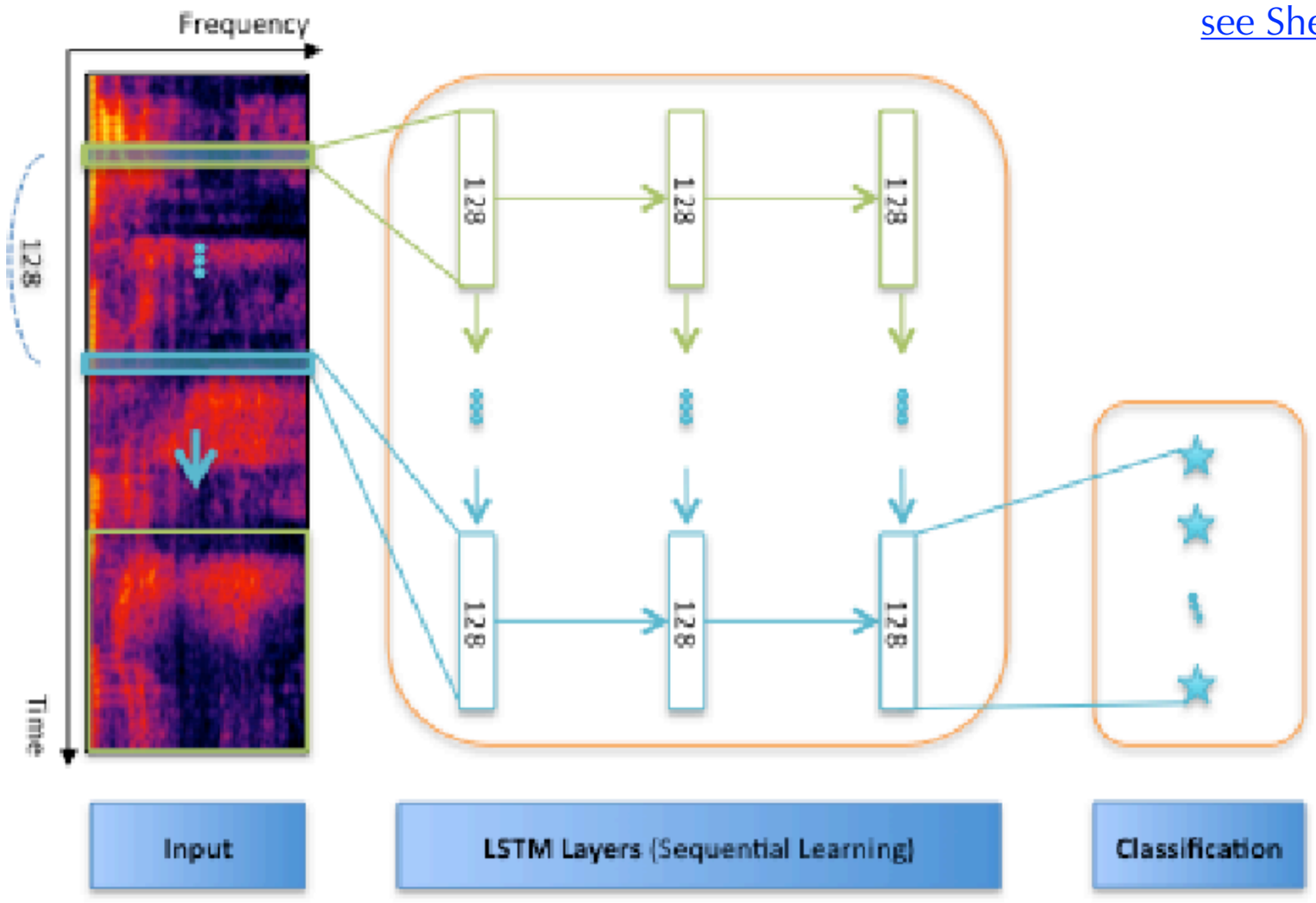


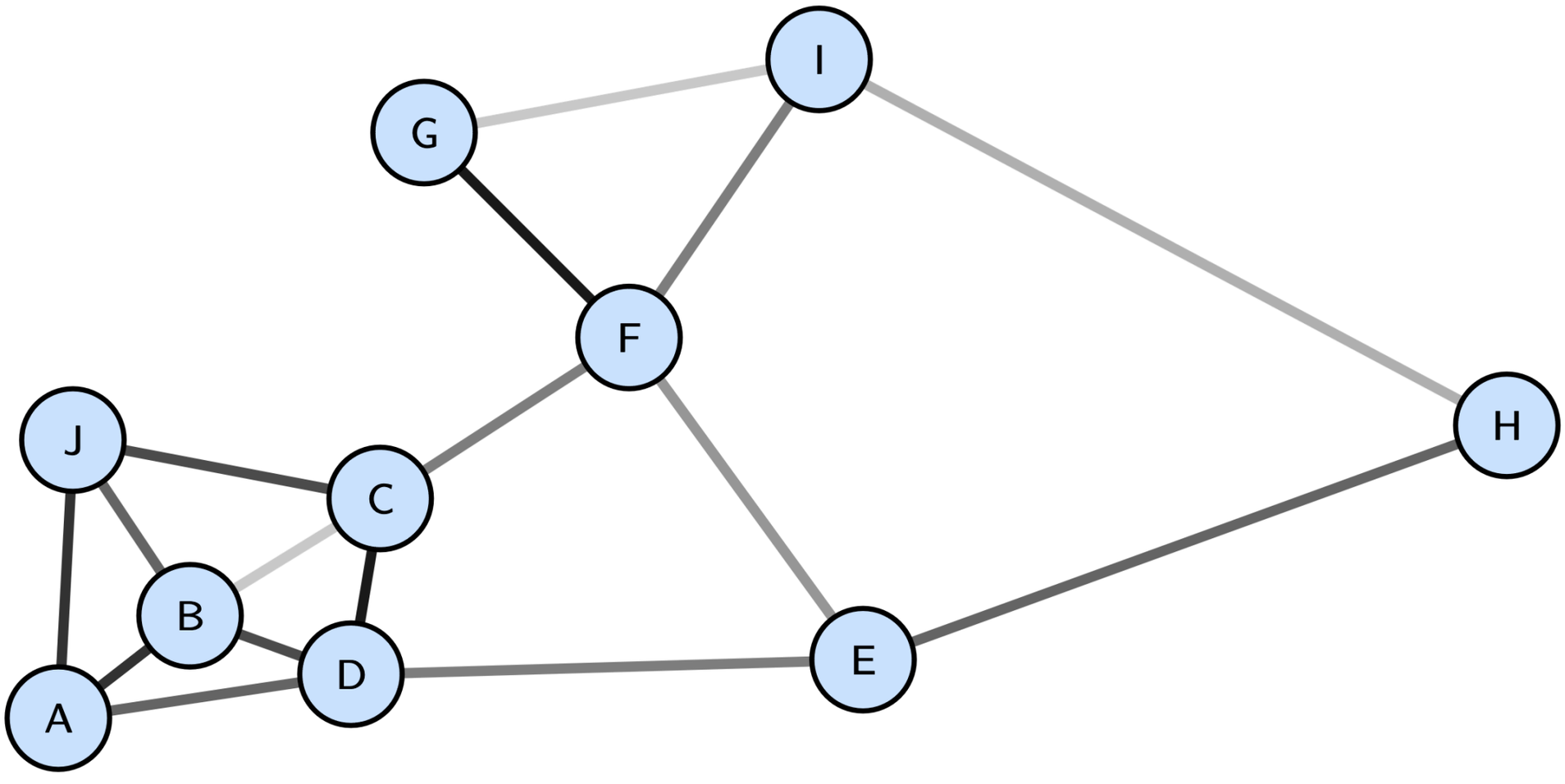
Fig. 4. The proposed LSTM structure for speech emotion recognition

W. Lim et al, 2016

Graph Neural Networks

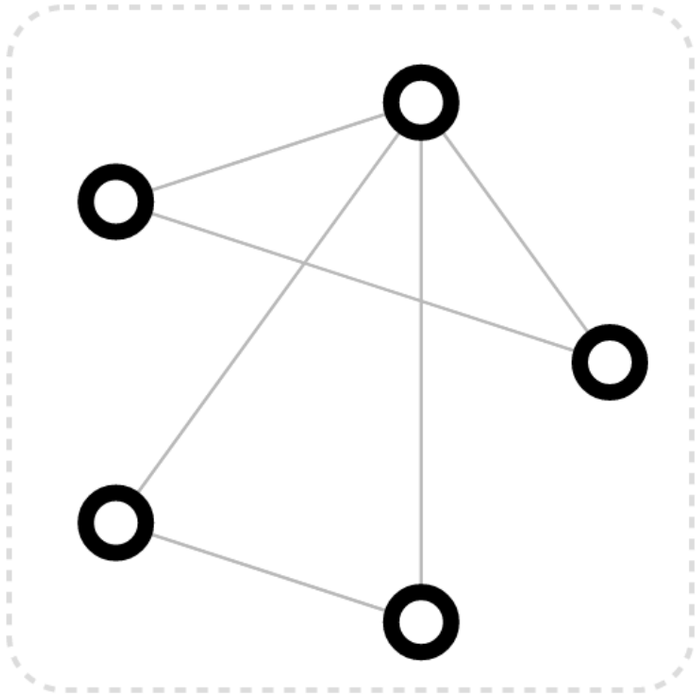
Graph data representation

- Data discussed so far had a fixed-size and/or regular-structured connection which we designed appropriate NN architectures to operate on
- What if data have more complex dependencies — i.e. they are connected over a more abstract not-fixed dimension
- **Let's represent the data as a graph and let a neural network learn the actual dimensions that connect the points**



What is a graph?

- A graph $\mathcal{G} = (\mathbf{g}, \mathcal{V}, \mathcal{E})$ represents relational data
  - Entities → **Nodes** $v \in \mathcal{V}$ with features $\mathbf{x}_v \in \mathbb{R}^{d_{\mathcal{V}}}$



V Vertex (or node) attributes
e.g., node identity, number of neighbors

E Edge (or link) attributes and directions
e.g., edge identity, edge weight

U Global (or master node) attributes
e.g., number of nodes, longest path

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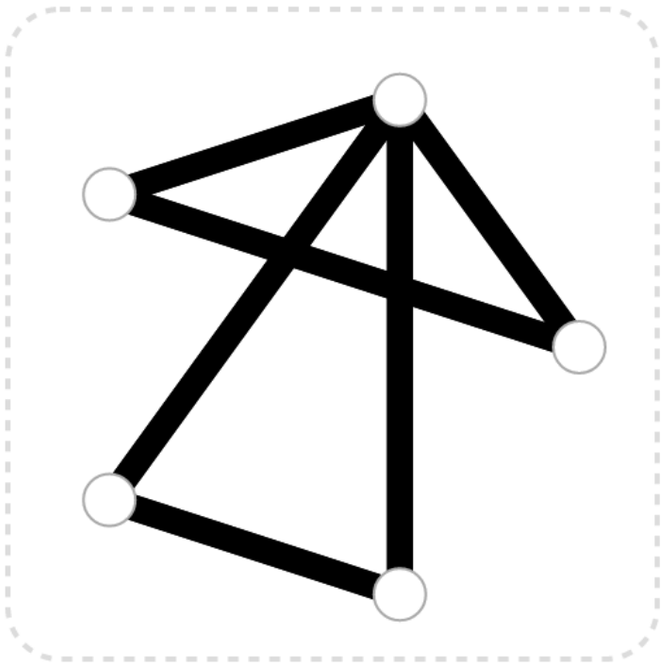
  - Relations → **Edges** $(u, v) \in \mathcal{E}$ with features $\mathbf{e}_{uv} \in \mathbb{R}^{d_{\mathcal{E}}}$

Edges define the pairs of nodes that exchange information

*Information coming from multiple edges must be **"aggregated"** at the source node*



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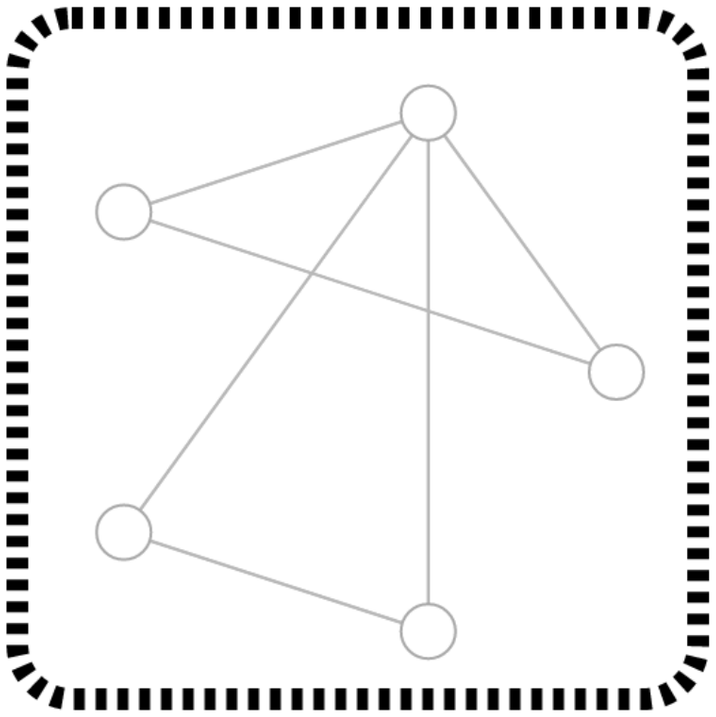
  - Global graph features $\mathbf{g} \in \mathbb{R}^d$



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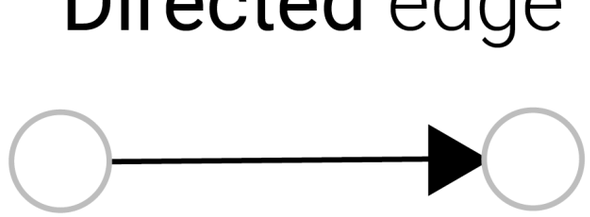
What is a graph?

We can can additionally specialize graphs by associating directionality to edges:

Undirected edge

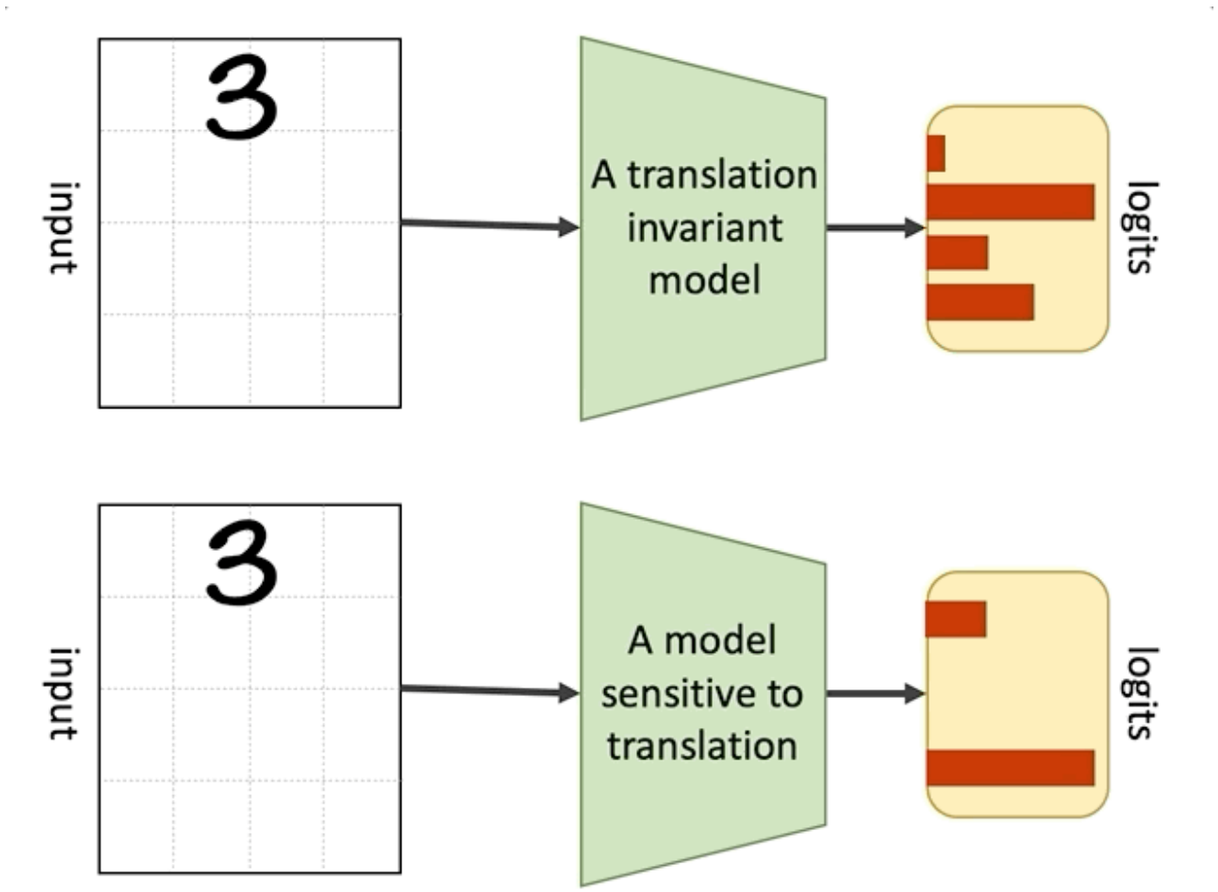
Directed edge



The edges can be directed, where an edge e has a source node, v_{src}, and a destination node v_{dst}. In this case, information flows from v_{src} to v_{dst}. They can also be undirected, where there is no notion of source or destination nodes, and information flows both directions. Note that having a single undirected edge is equivalent to having one directed edge from v_{src} to v_{dst}, and another directed edge from v_{dst} to v_{src}.

Symmetries

- We have seen that convolutional neural networks respect translational invariance
- Patterns are interesting irrespective of where they are in the image
- **Locality:** neighbouring pixels relate much more strongly than distant ones
- What about arbitrary graphs?



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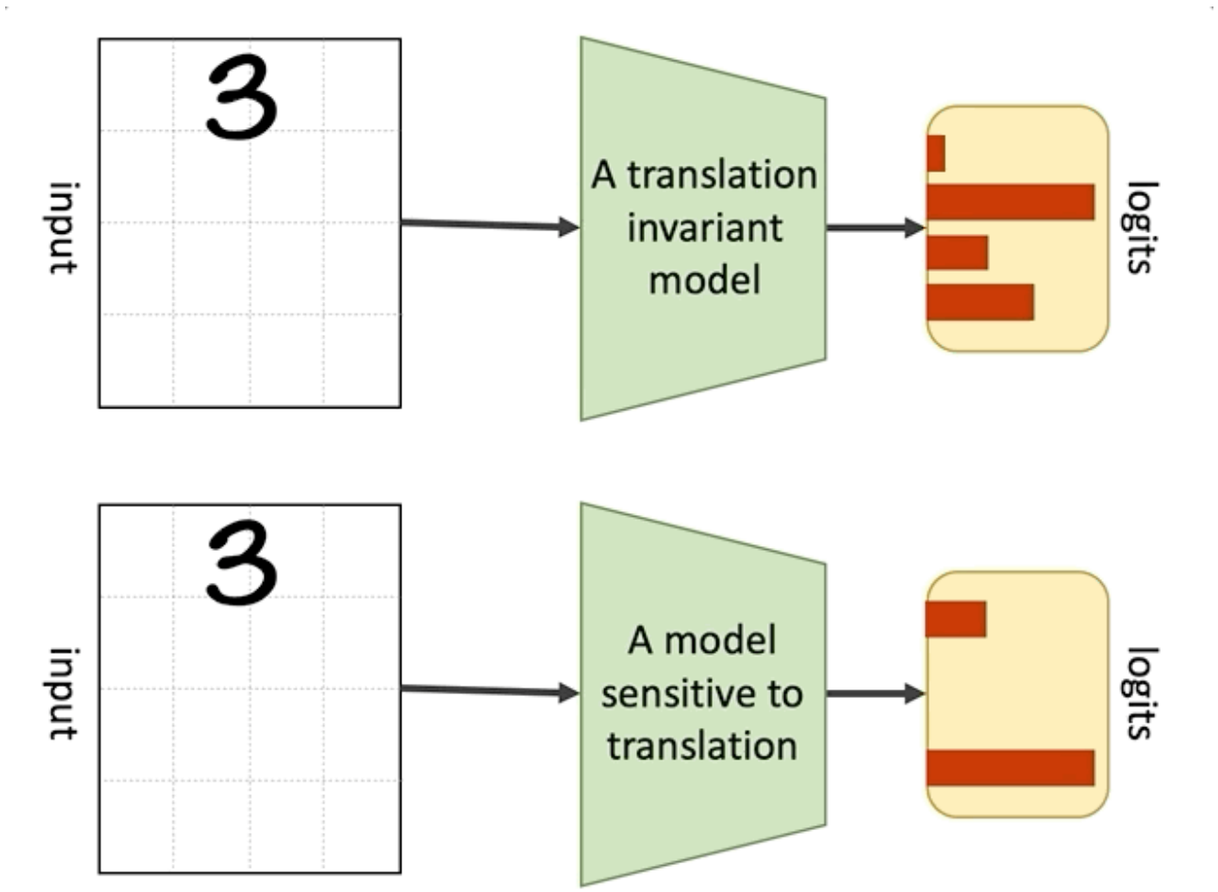
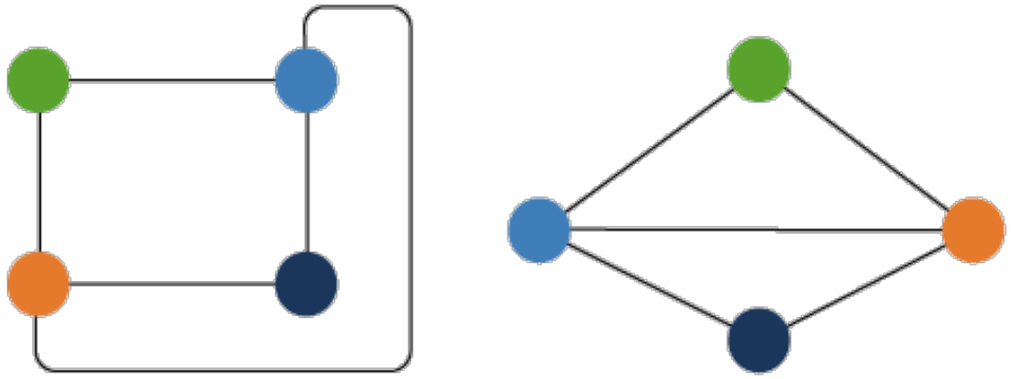
- **Locality:** neighbouring pixels relate much more strongly than distant ones
- What about arbitrary graphs?



Symmetries

- The nodes of a graph are not assumed to be in any order
- That is, we would like to get the same results for two isomorphic graphs



- To see how to enforce this, we'll go through some formalism…

Learning on sets: setup

- For now, assume the graph **has no edges** (e.g. set of nodes $\mathcal{V}$)
- Let $\mathbf{x}_i \in \mathbb{R}^k$ be the features of node i for $i = 1,2,...,n$
- We can stack them into a node feature matrix of shape $n \times k$:

$$\mathbf{X} = (\mathbf{x}_1, \mathbf{x}_2, \ldots, \mathbf{x}_n)^{\mathrm{T}}$$

- That is, the i**th** row of $\mathbf{X}$ corresponds to the feature vector $\mathbf{x}_i$ of node i
- Note that, by doing so, we have specified a **node ordering**!
  - We would like the result of any neural networks to not depend on this

Permutations

- Operations that change the node order are called **permutations** (there are **n!** of them)
  - e.g., a permutation (2, 4, 1, 3) means $\mathbf{y}_1 \leftarrow \mathbf{x}_2$, $\mathbf{y}_2 \leftarrow \mathbf{x}_4$, $\mathbf{y}_3 \leftarrow \mathbf{x}_1$, $\mathbf{y}_4 \leftarrow \mathbf{x}_3$
- To stay within linear algebra, each permutation defines an $n \times n$ matrix
  - such matrices are called **permutation matrices**
  - they have exactly one 1 in every row and column, and zeros everywhere else
  - their effect when left-multiplied is to permute the rows of $\mathbf{X}$, as

$$\mathbf{P}_{(2,4,1,3)}\mathbf{X} = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix} = \begin{bmatrix} \mathbf{x}_1 \\ \mathbf{x}_2 \\ \mathbf{x}_3 \\ \mathbf{x}_4 \end{bmatrix} = \begin{bmatrix} \mathbf{x}_2 \\ \mathbf{x}_4 \\ \mathbf{x}_1 \\ \mathbf{x}_3 \end{bmatrix}$$

Permutation *invariance*

- Eventually we want to solve tasks (e.g., classification) over graph data through a NN
- This means defining a function $f(x)$ over sets that will not depend on the order (which we want to preserve)
- Equivalently, applying a permutation matrix shouldn't modify the result!
- We arrive at a useful notion of **permutation invariance** — we say that $f(\mathbf{X})$ is permutation invariant if, for all permutation matrices $\mathbf{P}$ if

$$f(\mathbf{PX}) = f(\mathbf{X})$$

- One very generic form is the *Deep Sets* models [Zaheer at al., NeurIPS '17]:

$$f(\mathbf{X}) = \phi(\sum_{i \in \mathcal{V}} \psi(\mathbf{x}_i))$$

  - where ψ and ϕ are (learnable) functions, e.g. MLPs.
  - the **sum** aggregation is critical! (other choices possible, e.g. **max** or **avg**)

Permutation *equivariance*

- Permutation-invariant models are the optimal way to obtain graph-level outputs
- What if we would like answers at the **node** level?
- We seek functions that if we permute the nodes, it doesn't matter if we do it before or after the function
- Accordingly we say that $f(\mathbf{X})$ is **permutation equivariant** if, for all permutation matrices $\mathbf{P}$:

$$f(\mathbf{PX}) = \mathbf{P}f(\mathbf{X})$$

Permutation symmetries

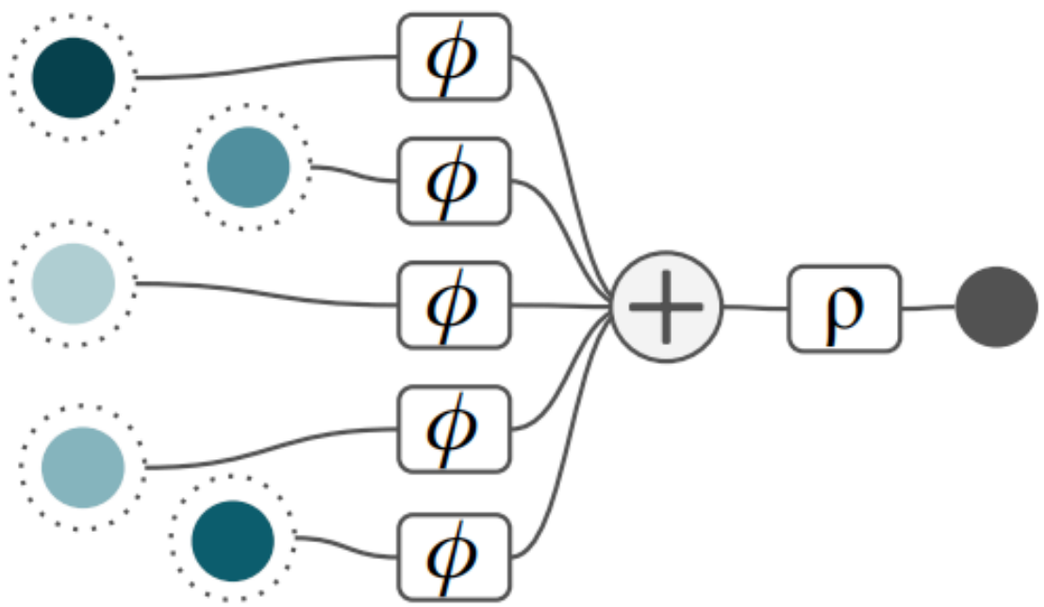
- The ϕ's transform each node inputs into a latent vector of lower dimension → this is called "*embedding*"

- **Permutation invariance:** if I change the order of the nodes the output of the output does not change

  - ensured by having a permutation invariant aggregation function like the **sum**

- **Permutation equivariance =** if I change the order of the nodes the output of ϕ's does not change

  - ensured by having the same function ϕ per each node embedding (i.e., sharing of weights)

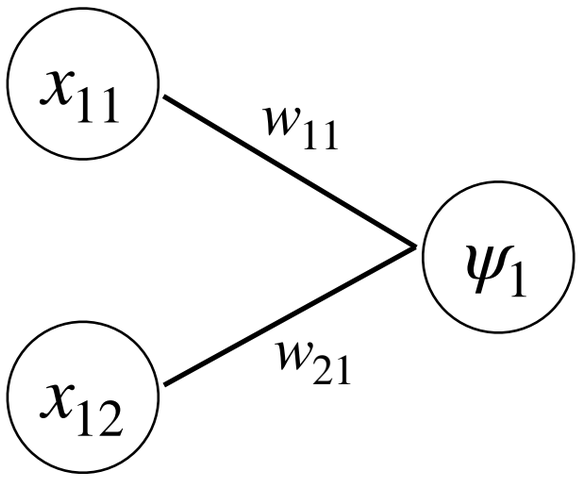


Numerical example

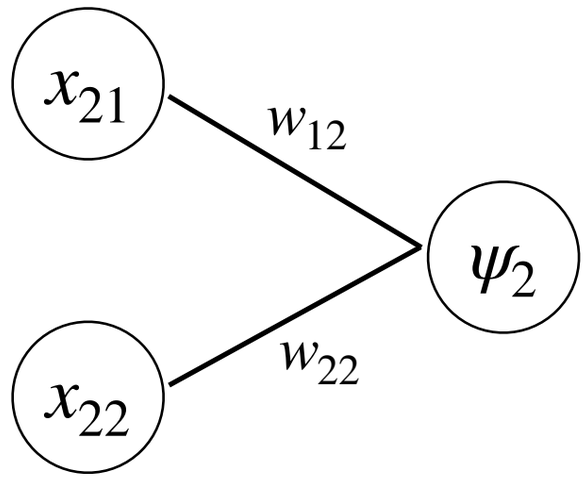
- We have two nodes made of two features:
  - node 1 has features $x_{11} = 3$ and $x_{12} = 4$
  - node 2 has features $x_{21} = 6$ and $x_{22} = 7$

$$f(\mathbf{X}) = \phi\left(\sum_{i \in \mathcal{V}} \psi(\mathbf{x}_i)\right)$$

- The functions ψ_1 and ψ_2 are two distinct MLPs that take as input the two features of the respective node and output two different nodes (= latent representation)



MLP ψ_1 has weights:
$w_{11} = 1$, $w_{21} = 2$



MLP ψ_2 has weights:
$w_{12} = 3$, $w_{22} = 4$

Numerical example

- So we now compute the ψ_i functions:

$$\psi_1 = w_{11}x_{11} + w_{12}x_{12} = 1 \times 3 + 2 \times 4 = 11$$

$$\psi_2 = w_{12}x_{21} + w_{22}x_{22} = 3 \times 6 + 4 \times 7 = 46$$

- And the final sum: $\psi_1 + \psi_2 = 11 + 46 = 57$

- If I exchange ψ_1 and ψ_2 the sum does not change … it would still gives $46 + 11 = 57$

- What if exchange the inputs? i.e. node 1 gets the features of node 2:

$$\psi_1 = w_{11}x_{11} + w_{12}x_{12} = 1 \times 6 + 2 \times 7 = 20$$

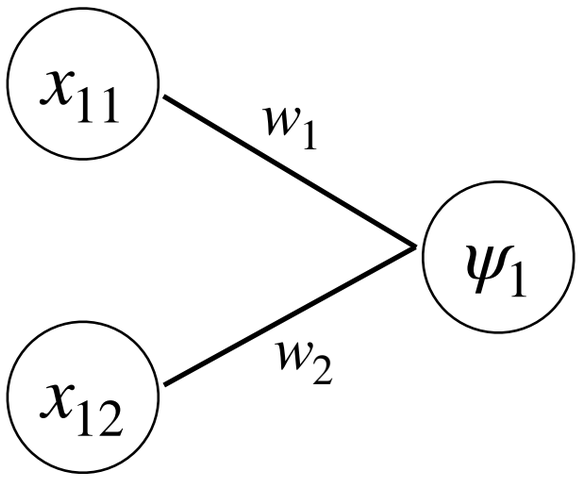
$$\psi_2 = w_{12}x_{21} + w_{22}x_{22} = 3 \times 3 + 4 \times 4 = 25$$

- The final sum is now: $\psi_1 + \psi_2 = 20 + 25 = 45$!!!

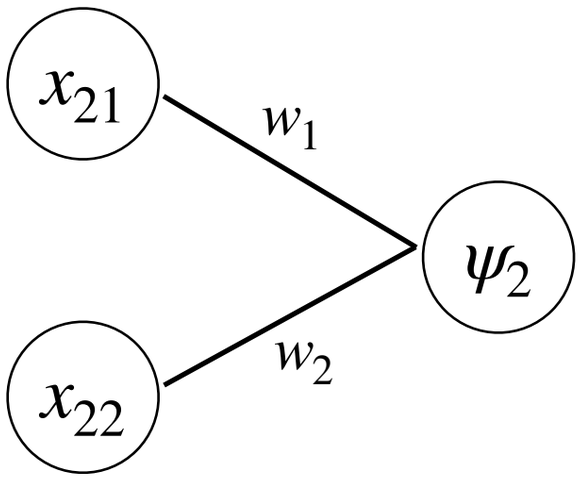
- **Therefore the full function is permutation invariant but not equivariant!**

Numerical example

- Now let's instead assume that $\psi_1 = \psi_2$, i.e. they share the same weights:
  - $w_{11} = w_{12} = w_1 = 3$
  - $w_{21} = w_{22} = w_2 = 4$



MLP ψ_1 has weights:
$w_1 = 3$, $w_2 = 4$



MLP ψ_2 has weights:
$w_1 = 3$, $w_2 = 4$

Numerical example

- So we now compute the ψ_i functions:

$$\psi_1 = w_1 x_{11} + w_2 x_{12} = 3 \times 3 + 4 \times 4 = 25$$

$$\psi_2 = w_1 x_{21} + w_2 x_{22} = 3 \times 6 + 4 \times 7 = 46$$

- And the final sum: $\psi_1 + \psi_2 = 25 + 46 = 71$

- If I exchange ψ_1 and ψ_2 the sum does not change … it would still gives $46 + 25 = 71$

- What if exchange the inputs? i.e. node 1 gets the features of node 2:

$$\psi_1 = w_1 x_{11} + w_2 x_{12} = 3 \times 6 + 4 \times 7 = 46$$

$$\psi_2 = w_1 x_{21} + w_2 x_{22} = 3 \times 3 + 4 \times 4 = 25$$

- The final sum is now: $\psi_1 + \psi_2 = 46 + 25 = 71$!!!

- **Therefore the full function is permutation invariant and also equivariant!**

Learning on graphs

- Now we augment the set of nodes with edges $\mathscr{E}$ between them
- We can represent these edges with an **adjacency matrix**, $\mathbf{A}$, such that:

$$a_{ij} = \begin{cases} 1 & \text{if } (i,j) \in \mathscr{E} \\ 0 & \text{otherwise} \end{cases}$$

- Further additions (e.g. edge features) are possible but ignored for simplicity
- Our main desire for permutation {in,equi}variance still holds!

Learning on graphs

- The main difference: node permutations now also accordingly act on the edges
- We need to appropriately permute both rows and columns of $\mathbf{A}$
  - when applying a permutation matrix $\mathbf{P}$, this amounts to $\mathbf{P}\mathbf{A}\mathbf{P}^{\mathrm{T}}$
- We arrive at updated definitions of suitable functions $f(\mathbf{X}, \mathbf{A})$ over graphs:

Invariance: $f(\mathbf{P}\mathbf{X}, \mathbf{P}\mathbf{A}\mathbf{P}^{\mathrm{T}}) = f(\mathbf{X}, \mathbf{A})$

Equivariance: $f(\mathbf{P}\mathbf{X}, \mathbf{P}\mathbf{A}\mathbf{P}^{\mathrm{T}}) = \mathbf{P}f(\mathbf{X}, \mathbf{A})$

Locality on graphs

- On a graph, we enforced equivariance by applying the same function to every node in isolation

- Graphs give us a broader context: a node's **neighbourhood**

  - for a node i, its (1-hop) neighbourhood is commonly defined as follows:

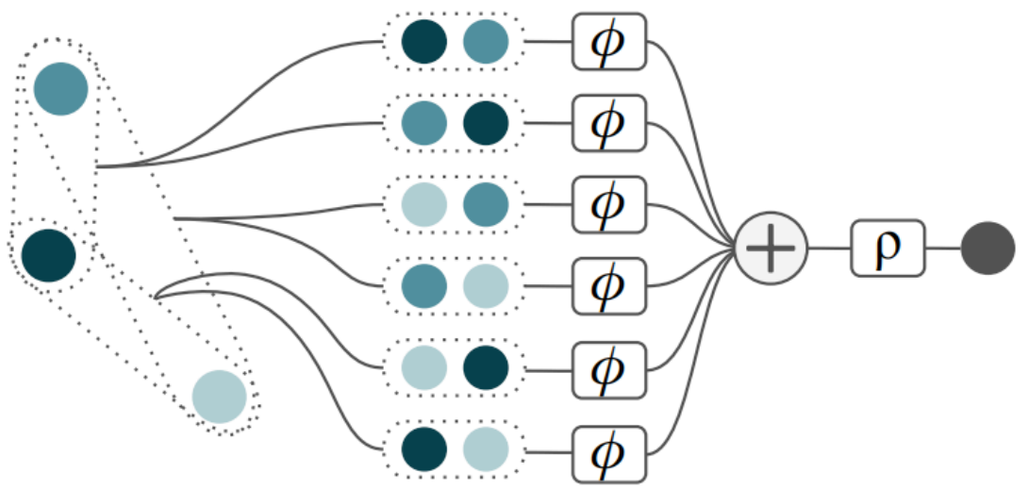
$$\mathcal{N}_i = \{j : (i,j) \in \mathcal{E} \vee (j,i) \in \mathcal{E}\}$$

  - i.e. all nodes that have edges starting at i plus all the nodes that are directed to i

- Accordingly, we can use the multiset of features in the neighbourhood

$$\mathbf{X}_{\mathcal{N}_i} = \{\mathbf{x}_j \ : \ j \in \ \mathcal{N}_i\}$$

  - by defining a local function, g,
    as operating over this multiset: $g(\mathbf{x}_i, \mathbf{X}_{\mathcal{N}_i})$



in this example every node is neighbour of each others but they share the same g

Graph Neural Networks

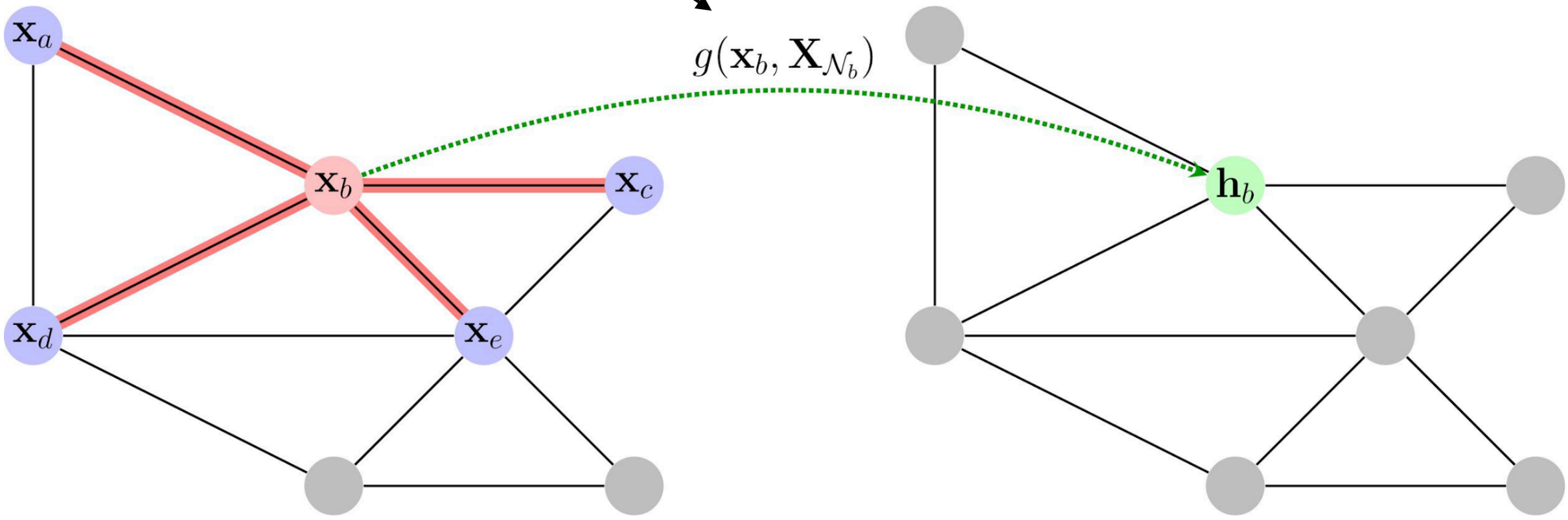
- Now we can construct permutation equivariant functions, $f(\mathbf{X}, \mathbf{A})$, by appropriately applying the same local function, g, over all neighbours

$$f(\mathbf{X}, \mathbf{A}) = \begin{bmatrix} g(\mathbf{x}_1, \mathbf{X}_{\mathcal{N}_1}) \\ g(\mathbf{x}_2, \mathbf{X}_{\mathcal{N}_2}) \\ \vdots \\ g(\mathbf{x}_n, \mathbf{X}_{\mathcal{N}_n}) \end{bmatrix}$$

- To ensure equivariance, we need g to not depend on the order of the vertices in $\mathcal{X}_{\mathcal{N}_i}$
  - Hence, g should be permutation invariant!

GNNs — how does that work?

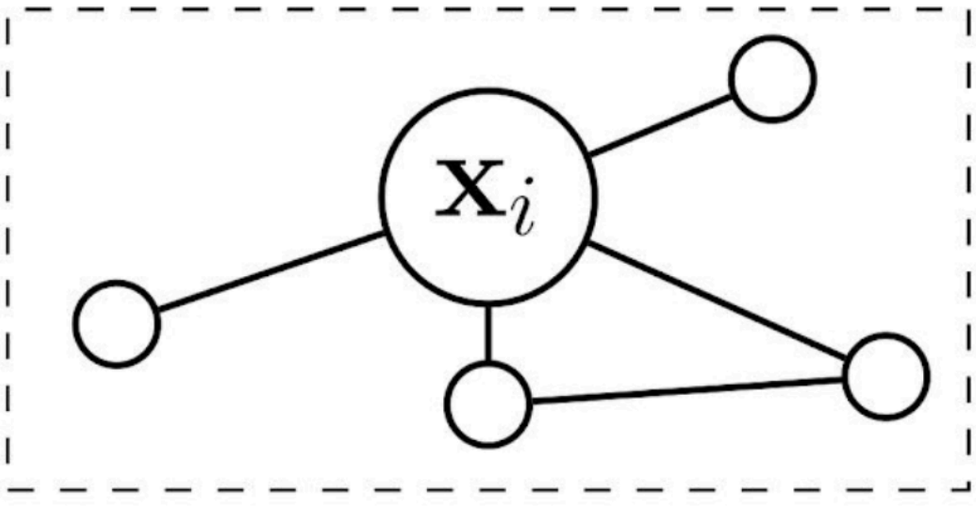
this is permutation invariant
ensuring equivariance of the full NN



$$\mathbf{X}_{\mathcal{N}_b} = \{\{\mathbf{x}_a, \mathbf{x}_b, \mathbf{x}_c, \mathbf{x}_d, \mathbf{x}_e\}\}$$

How to use GNNs?

- We start with nodes some of which have connections to others through the adjancency matrix → specified beforehand by edges



Inputs

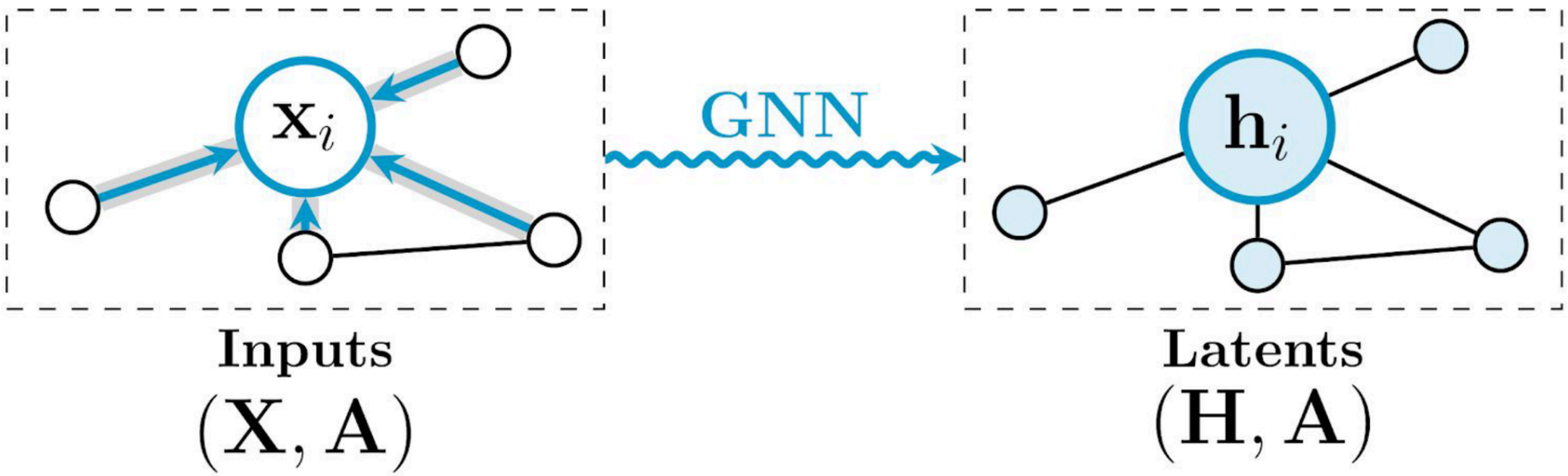
$(\mathbf{X}, \mathbf{A})$

How to use GNNs?

- We start with nodes some of which have connections to others through the adjancency matrix → specified beforehand by edges

- We let the connected nodes (through the edges) to transfer info to the source node $\mathbf{x}_i$ through an MLP (i.e. you learn what info from neighbours are important given $\mathbf{x}_i$)

  - this creates a new node representation $\mathbf{h}_i$ that takes into account features of neighbours



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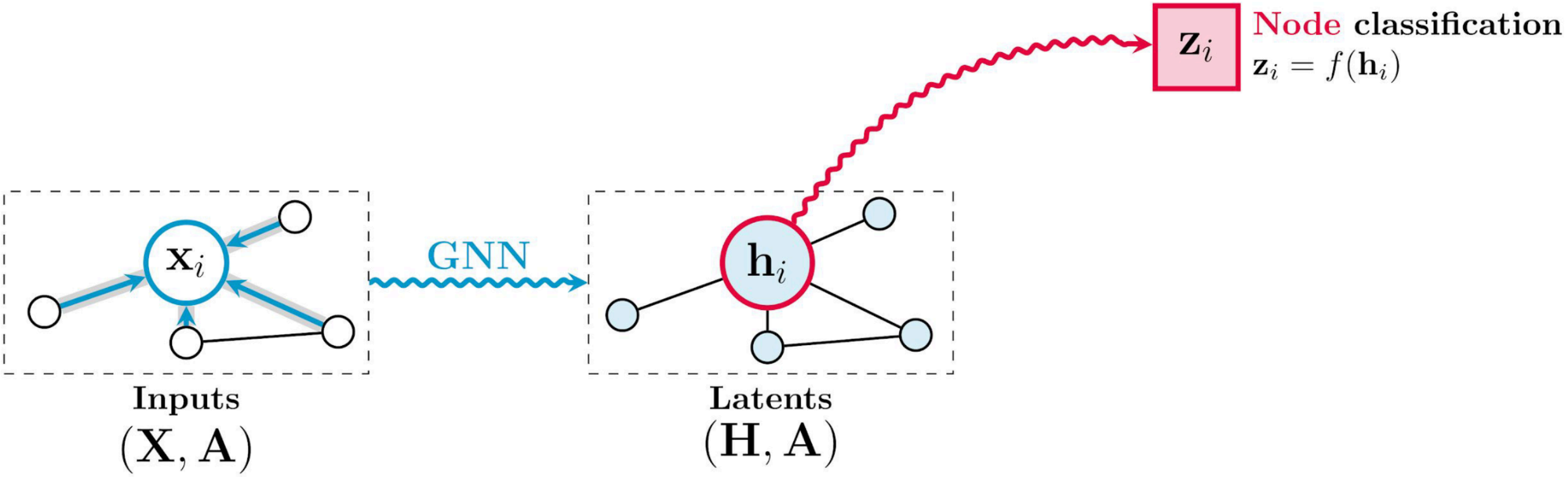
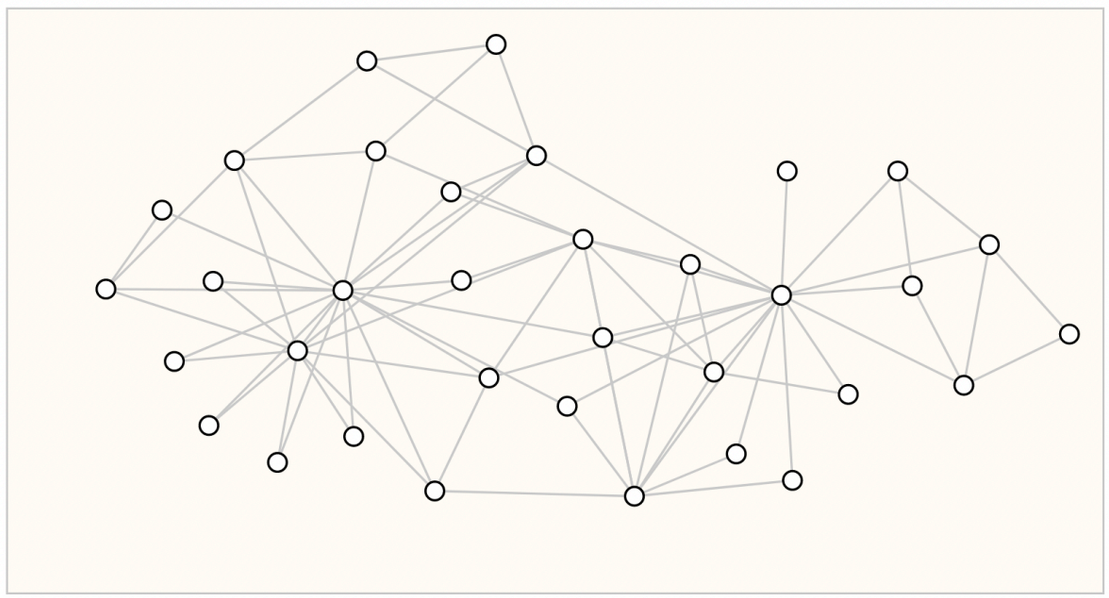


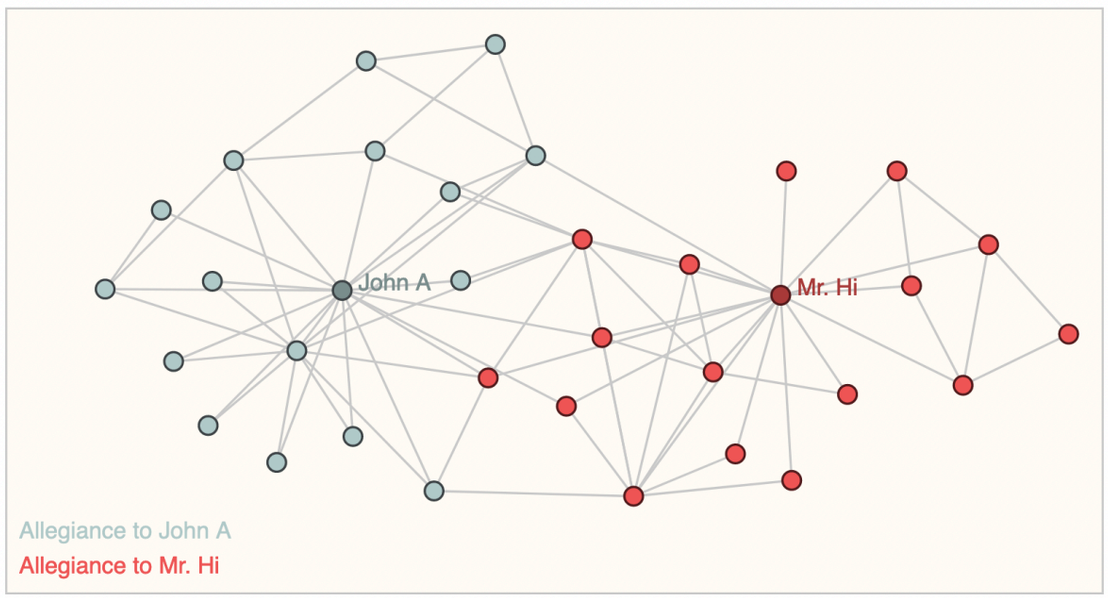
Tasks for graph data

- **Node-level task**: predict some property for each node in a graph
- Classic example: the Zach's karate club — a social network of a university karate club
  - a feud between Mr. Hi (Instructor) and John H (Administrator) creates a schism in the club
  - the task is to classify whether a given member becomes loyal to either Mr. Hi or John H
  - "distance" between a node to either the Instructor or Administrator is highly correlated to this label



Input: graph with unlabled nodes

→



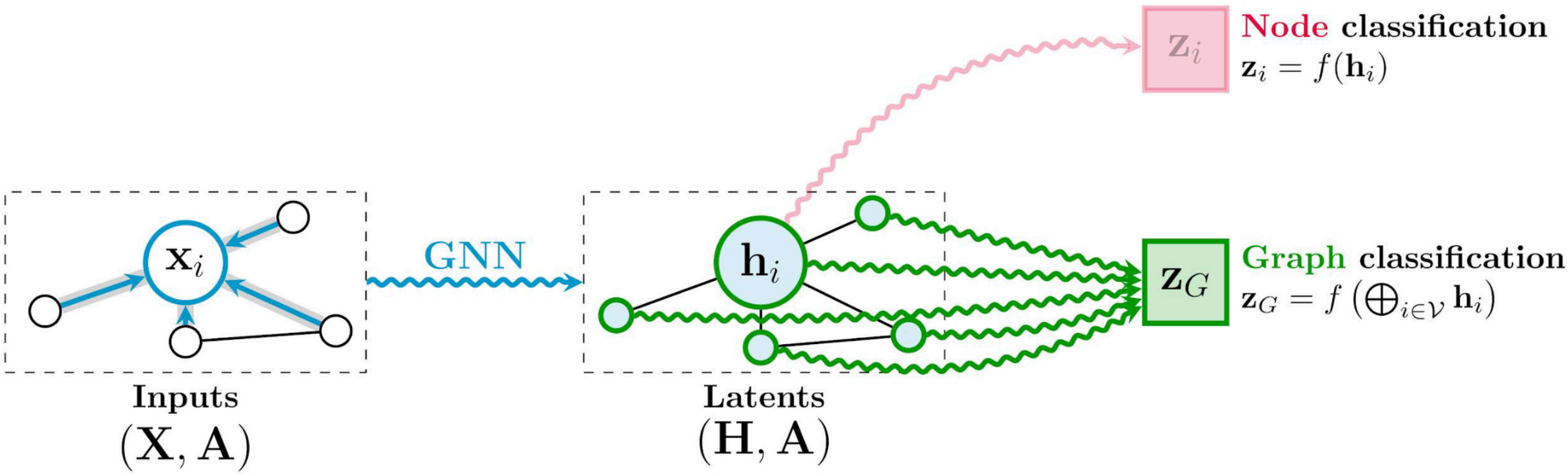
Output: graph node labels

How to use GNNs?

- We start with nodes some of which have connections to others through the adjancency matrix → specified beforehand by edges

- We let the connected nodes (through the edges) to transfer info to the source node $\mathbf{x}_i$ through an MLP (i.e. you learn what info from neighbours are important given $\mathbf{x}_i$)

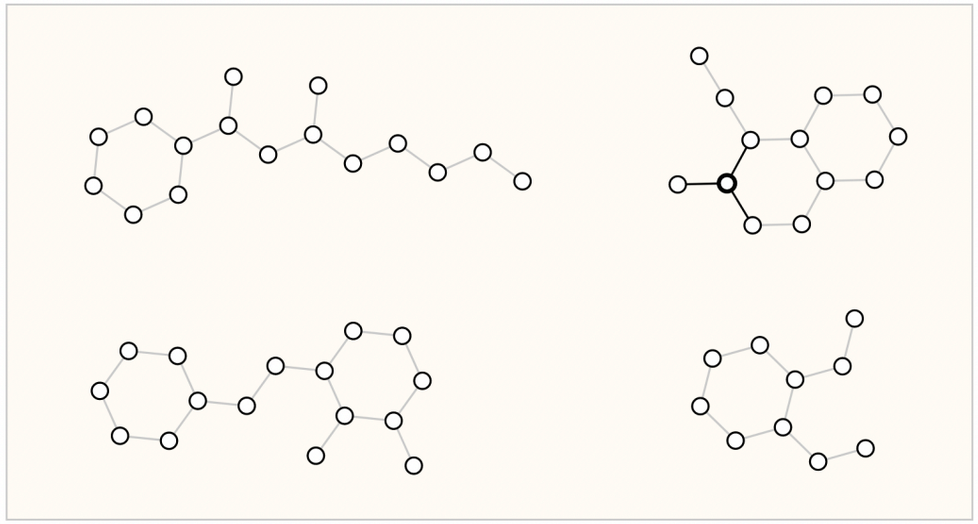
  - this creates a new node representation $\mathbf{h}_i$ that takes into account features of neighbours



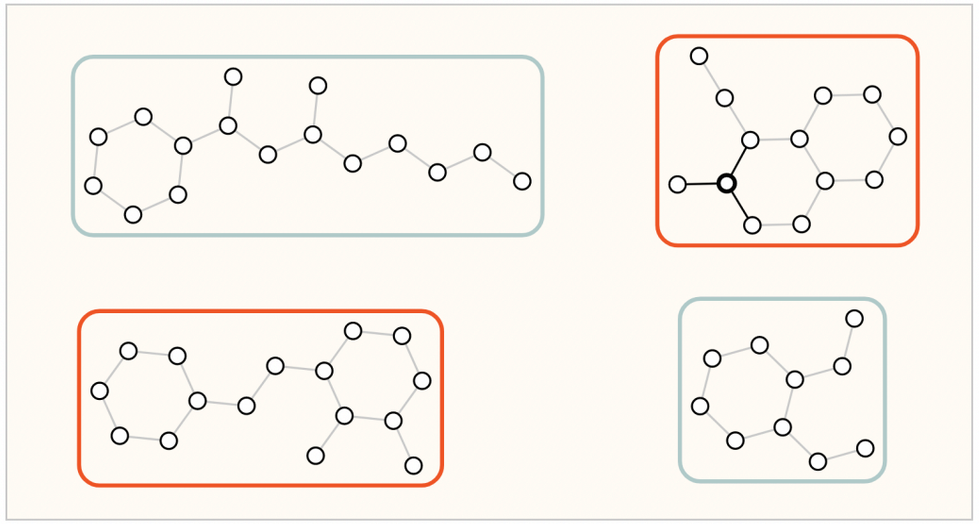
Tasks for graph data

- **Graph-level task:** predict some property for a whole graph

  - example: predict what the molecule smells like or whether it will bind to a receptor implicated in a disease



Input: graphs



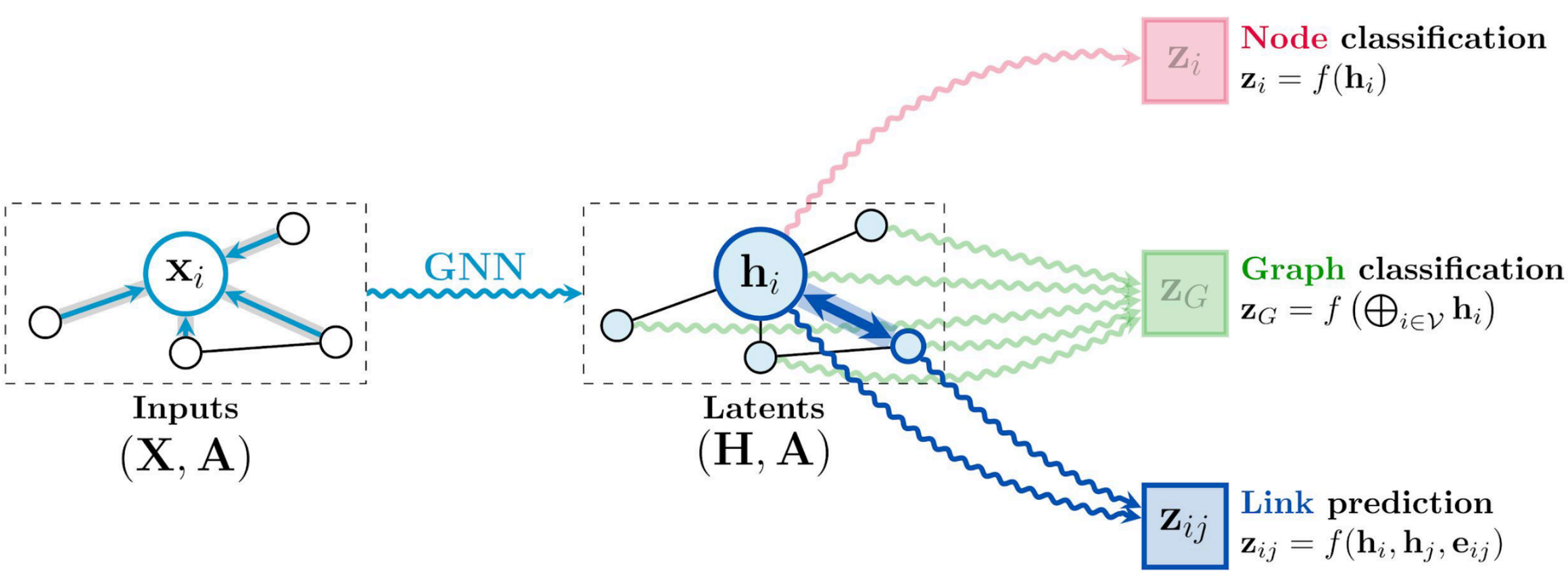
Output: labels for each graph, (e.g., "does the graph contain two rings?")

How to use GNNs?

- We start with nodes some of which have connections to others through the adjancency matrix → specified beforehand by edges

- We let the connected nodes (through the edges) to transfer info to the source node $\mathbf{x}_i$ through an MLP (i.e. you learn what info from neighbours are important given $\mathbf{x}_i$)

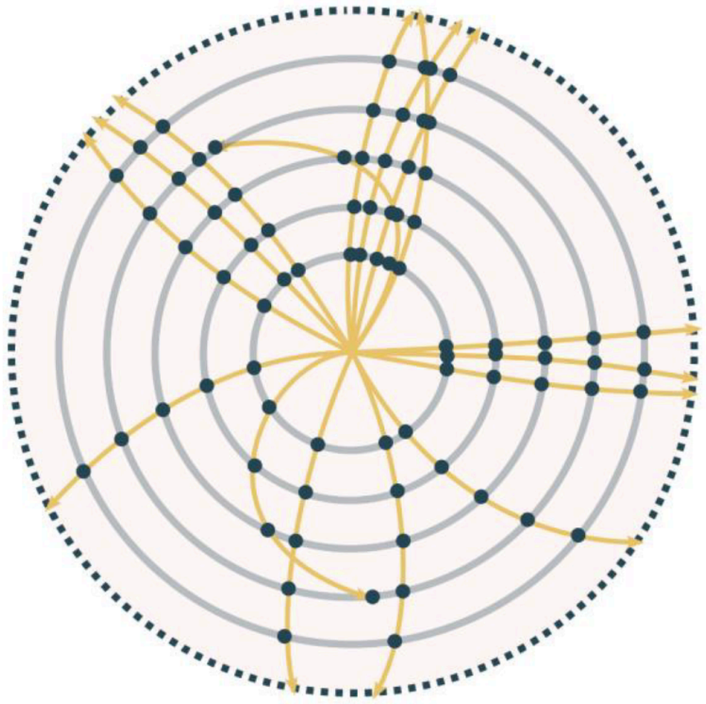
  - this creates a new node representation $\mathbf{h}_i$ that takes into account features of neighbours



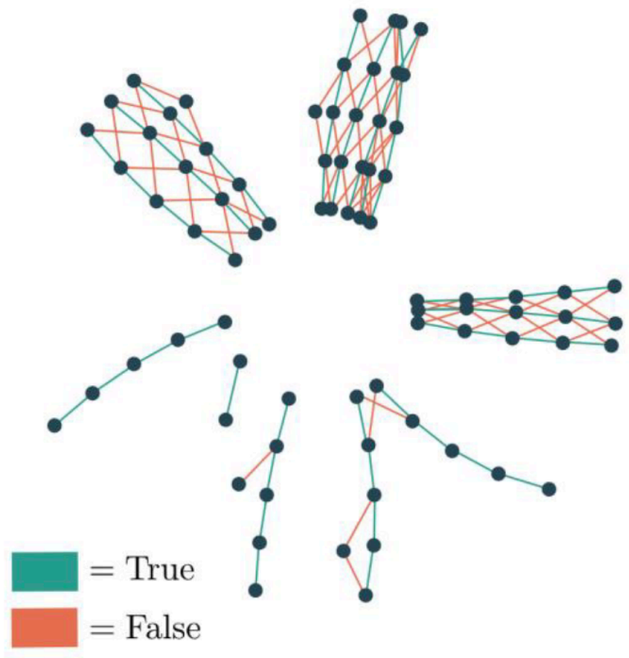
Tasks for graph data

- **Edge-level task:** predict some property or presence of edges in a graph
  - if we wish to discover connections between entities, we could consider the graph fully connected and based on their predicted value prune edges to arrive at a sparse graph

- Draw edges to hypothesize various particle trajectories, train a GNN to classify edges



Input data is a 3D *point cloud*



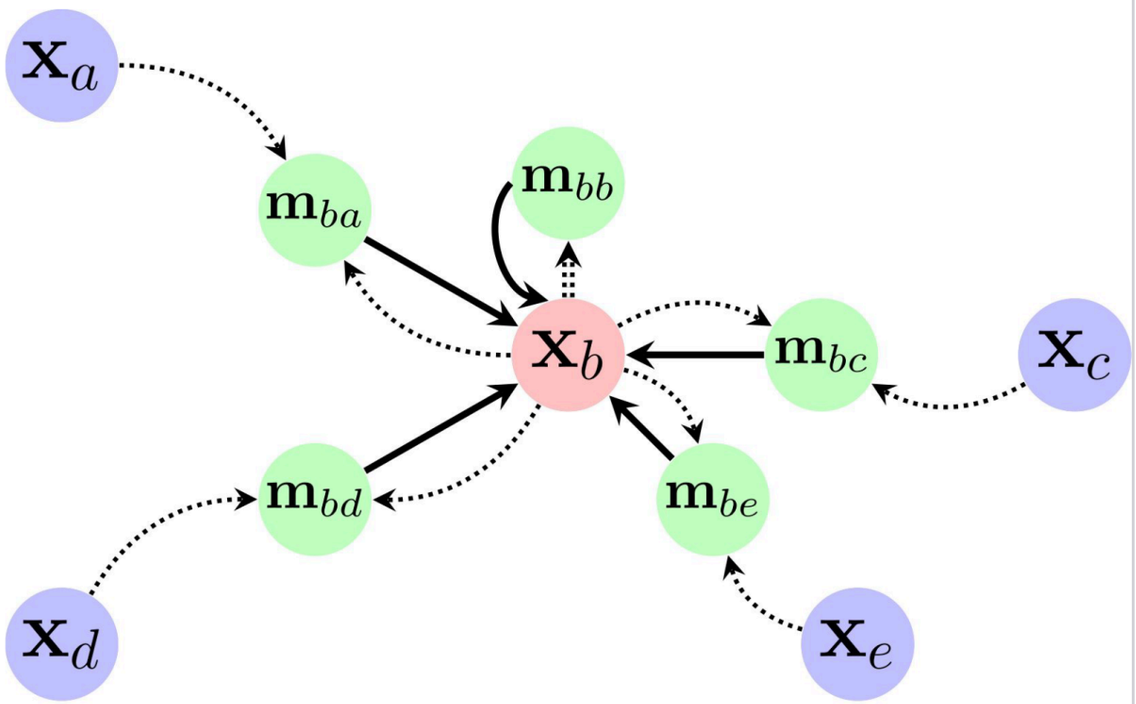
Train on graphs with edge truth labels

What's in a GNN layer?

- As mentioned, we construct permutation-equivariant functions $f(\mathbf{X}, \mathbf{A})$ over graphs by shared application of a local permutation-invariant
  - we often refer to f as "GNN layer", g as "diffusion", "propagation", "message passing"
- Now we look at ways in which we can actually concretely define g
  - Very intense area of research!
- This is the magic of GNNs — depending how you define g you can enforce basics (permutation) but also additional symmetries (*relational inductive bias*)
  - GNNs are very flexible!

Basic formalism of GNN

- The many GNN flavours are variants of a basic formalism called **Message Passing NN**



Message-passing

- **message passing**: for target node $i = b$, the "message" is passed at iteration k from neighbouring nodes a, c, d, e to the target node as

$$m_i^{(k)} = \sum_j M(h_i^{(k)}, h_j^{(k)}, e_{ij})$$

- Node feature update for the target node exploits all those info from neighbours as

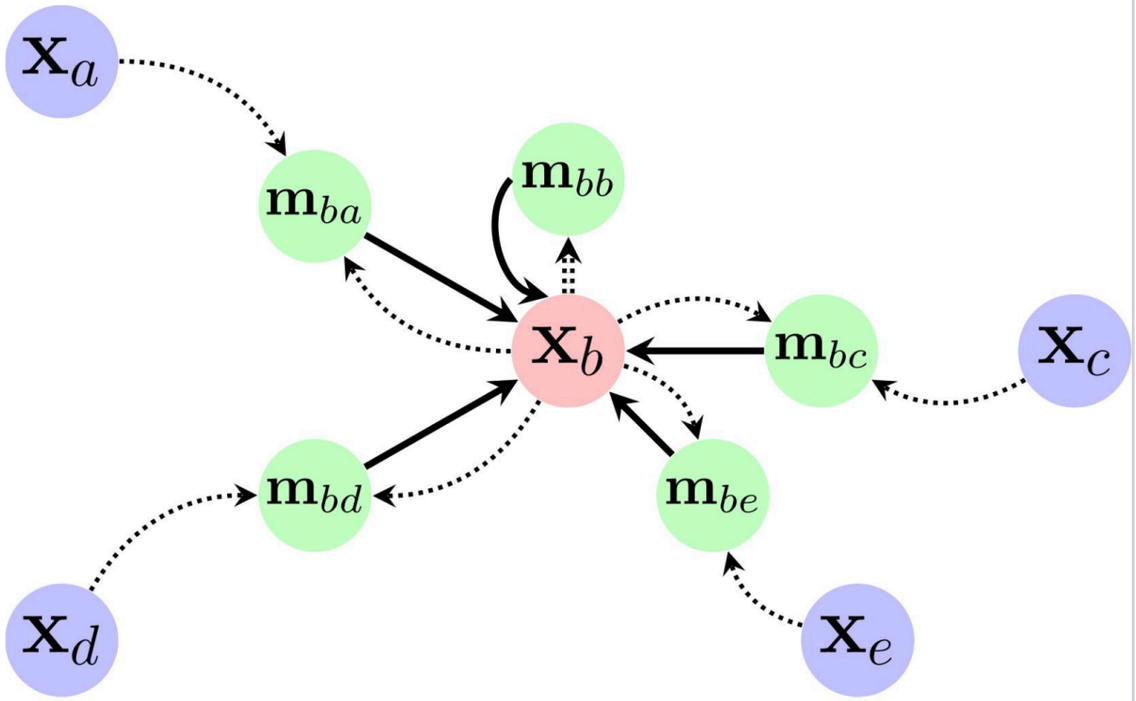
$$h_i^{(k+1)} = U(h_i^{(k)}, m_i^{(k)})$$

This is the basic GNN layer
If you stack more layers you get info from farther apart

- The functions M and U are message and updated functions
- The same can be performed on edges

Basic formalism of GNN

- The many GNN flavours are variants of a basic formalism called **Message Passing NN**



Message-passing

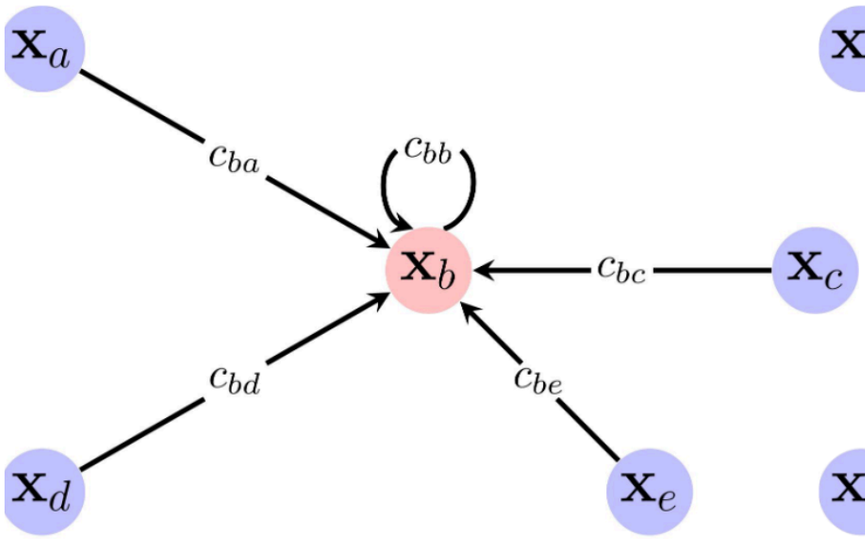
This is the basic GNN layer
If you stack more layers you get info from farther apart

$$m_i^{(k)} = \sum_j M(h_i^{(k)}, h_j^{(k)}, e_{ij})$$

$$h_i^{(k+1)} = U(h_i^{(k)}, m_i^{(k)})$$

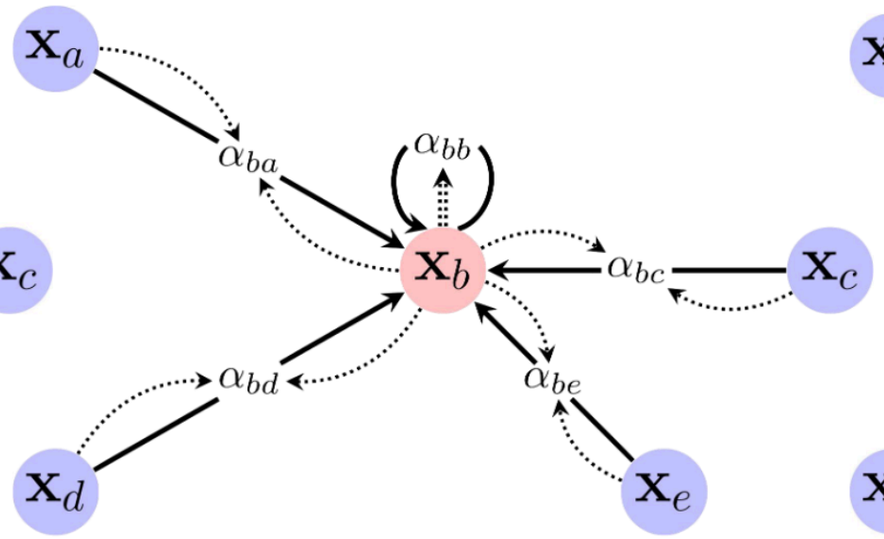
- The functions M and U are message and updated **functions**
  - can be simple MLPs in the simplest setup
  - must preserve permutation in/equivariance
- But depending on how these **functions** are designed one can incorporate different kinds of symmetries and assumptions
- This gives the different GNNs flavours

Basic "flavours" of GNNs



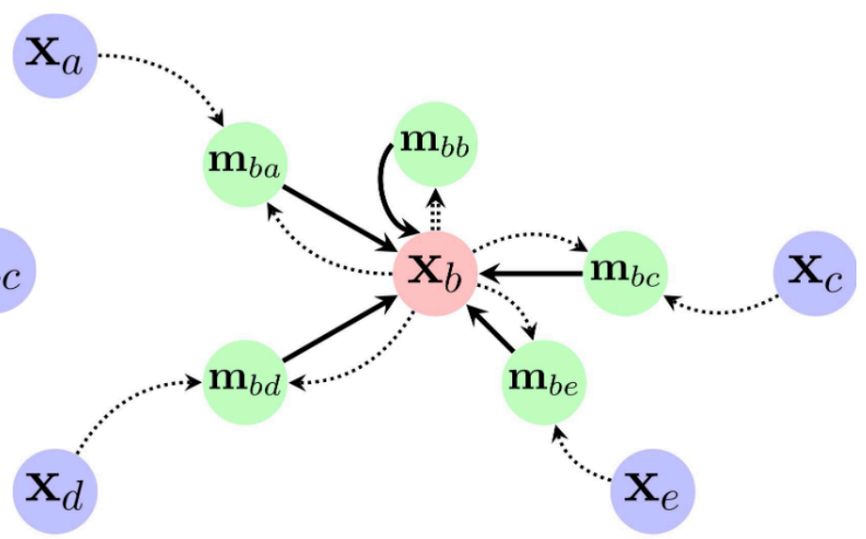
Convolutional

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} c_{ij}\psi(\mathbf{x}_j)\right)$$



Attentional

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} a(\mathbf{x}_i, \mathbf{x}_j)\psi(\mathbf{x}_j)\right)$$



Message-passing

$$\mathbf{h}_i = \phi\left(\mathbf{x}_i, \bigoplus_{j \in \mathcal{N}_i} \psi(\mathbf{x}_i, \mathbf{x}_j)\right)$$

Graph Convolutional NN

- In vanilla GCN the weight c_{ij} is a fixed value that normalize the the sum of the neighbour embeddings to make the aggregated message of the same size for all nodes

  - by using the sum as aggregation function you expect the output to be larger for nodes that have more neighbours → numerical instabilities

  - can be solved with the mean, i.e. c_{ij} = number of neighbours, but there are also other options

$$\mathbf{h}_u^{(k)} = \sigma\left(\mathbf{W}^{(k)} \sum_{v \in \mathcal{N}(u) \cup \{u\}} \frac{\mathbf{h}_v}{\sqrt{|\mathcal{N}(u)||\mathcal{N}(v)|}}\right)$$

node degree