CS 598CM: ML for Compilers and Architecture

Instructor: Charith Mendis



Paper Reviews

- Submit a 250-750 word summary of the paper including
 - Problem definition
 - Key contributions and solution overview
 - Evaluation summary
 - Strengths and weaknesses (limitations) of the technique(s)
- Let me know how you would extend the paper in 1-2 sentences (Can be vague and creative) => May be project ideas:)

Paper Presentation

- Presentations start on September 12th; assignments would be available today.
- Week before: Meet instructor in person or virtually to discuss the presentation plan (compulsory!)
 - Use this time to ask questions and discuss the outline
 - Presentation slides are due when reviews are due for that class
 - Submit the final slides using the form on website
 - You can use office hours for this or schedule a meeting with me
- During the class: Be present in class either in person or virtually (compulsory!)
 - Deliver a 20-30 min presentation on the paper
 - Answer questions for the following 15 min
 - Final 30 min for open discussion on the paper (lead by the instructor)

Paper Presentation

- After class: Summarize the discussion of the paper within 250 750 words
 - Submit the summary within 2 days at the end of the class
 - Update the same form to submit the summary (edit the same entry)
- The presentation should include
 - Problem definition
 - Motivation: Why is this an important problem?
 - Outline the high-level solution
 - Illustrate the solution
 - Evaluation: What worked and what didn't
 - Related Work: Put the solution in context of other research
 - Strengths and weaknesses
 - How would you extend this work?

Introductions!

- Let's get to know each other a second time!
- No specific format
 - Name
 - Department
 - Advisor
 - Research Project (if any)

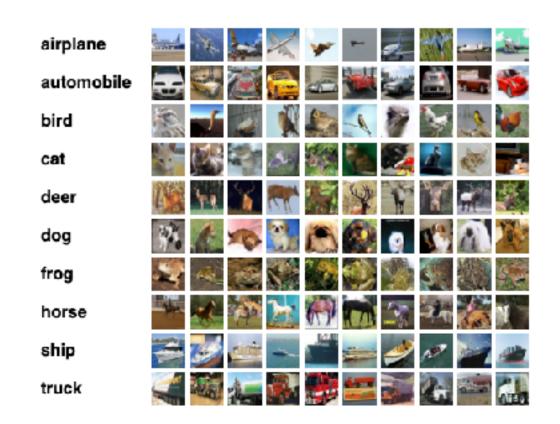
 Please drop by if you want to discuss exciting class projects (Email me before to check for availability)! Potentially leading to publication!

Recap

- Domain Specific Languages and Optimizations
 - XLA Operator Fusion, Graph Rewrites
 - Graph Processing
- ML in Architecture
 - Branch Prediction

Lecture 5: Machine Learning Techniques

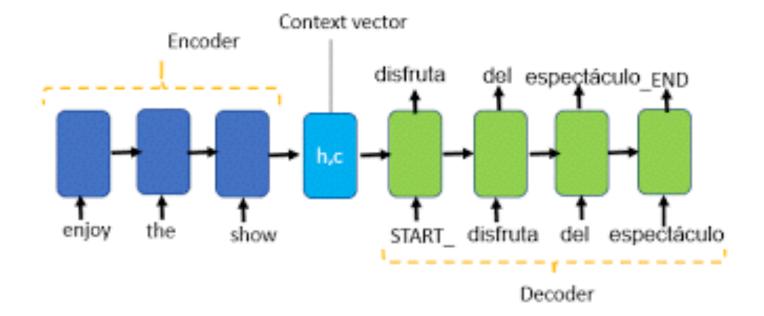
- Supervised Learning (labelled data)
- Unsupervised Learning
- Semi-supervised Learning
- Reinforcement Learning





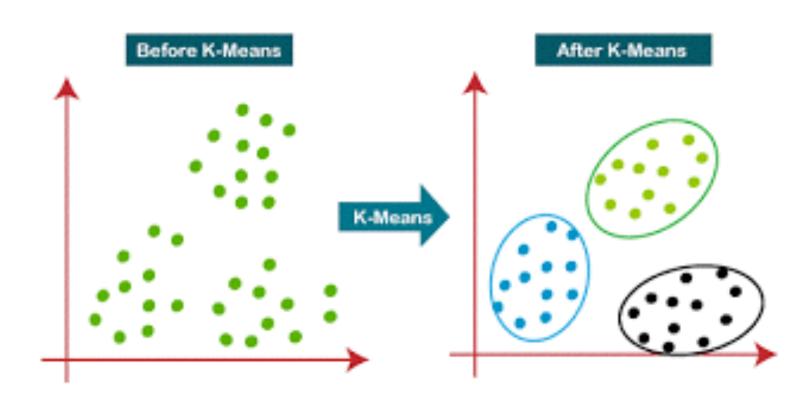
Object Detection

Image Classification

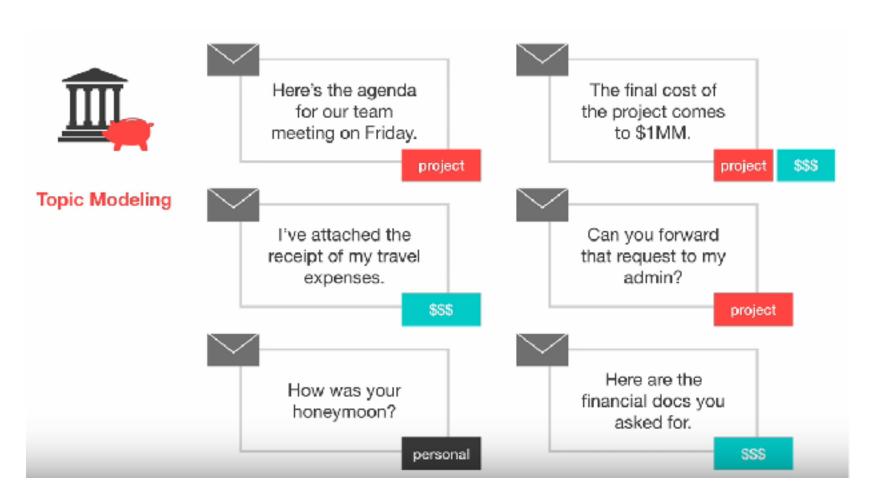


Machine Translation

- Supervised Learning
- Unsupervised Learning (unlabelled data)
- Semi-supervised Learning
- Reinforcement Learning



K-means clustering



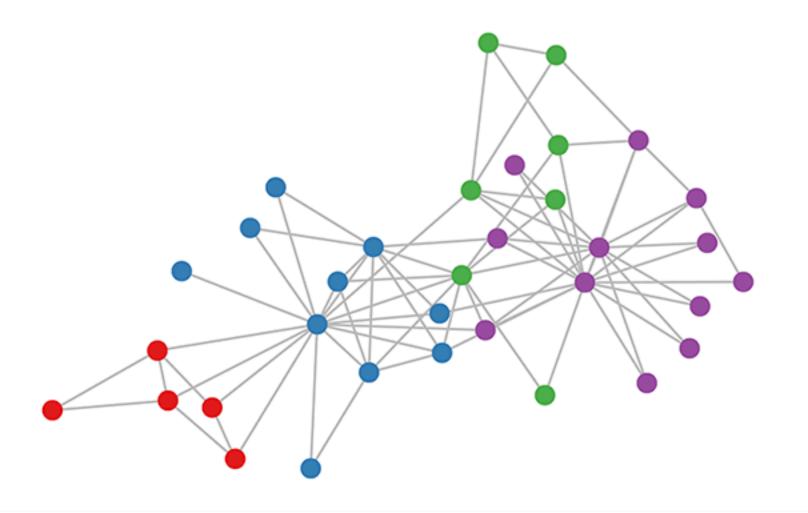
Topic Modeling

- Supervised Learning
- Unsupervised Learning
- Semi-supervised Learning
- Reinforcement Learning

Learning using a small number of labelled data and a large number of unlabelled data

Community Detection

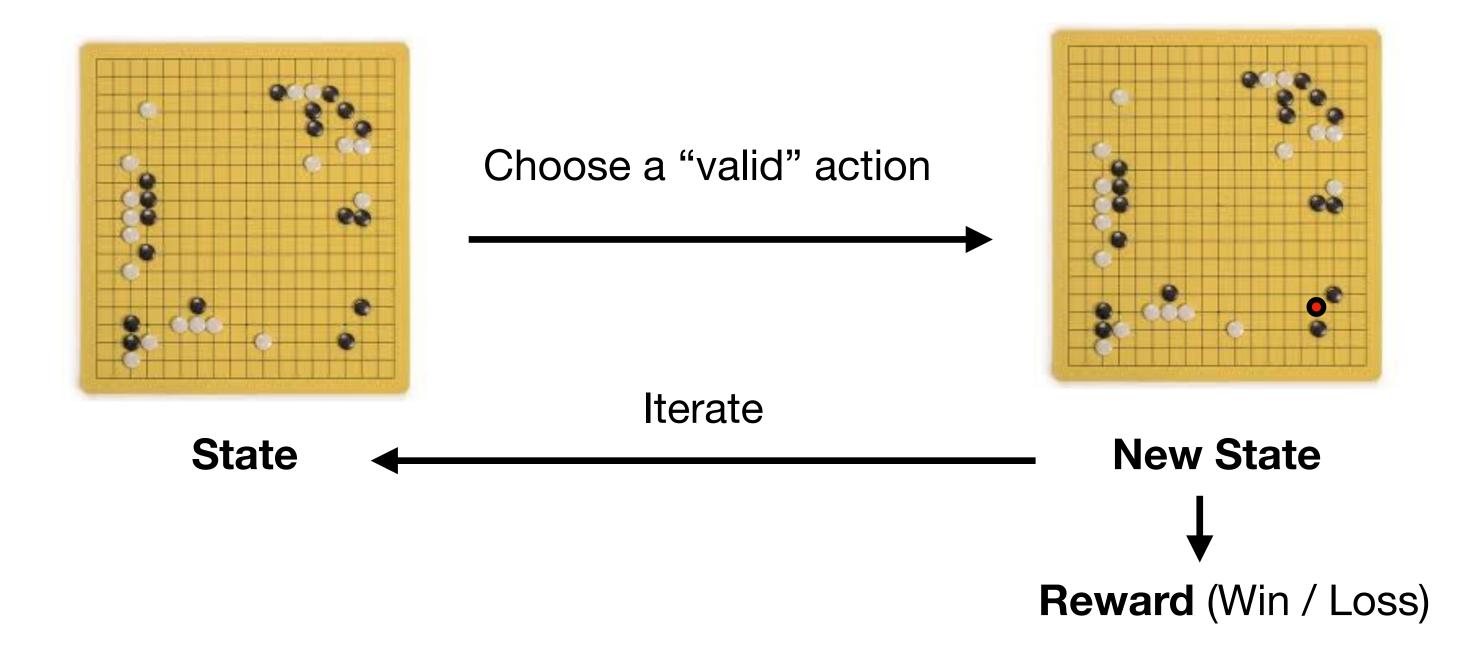
Node classification



Karate club graph, colors denote communities obtained via modularity-based clustering (Brandes et al., 2008).

No labelled data; learn from experience

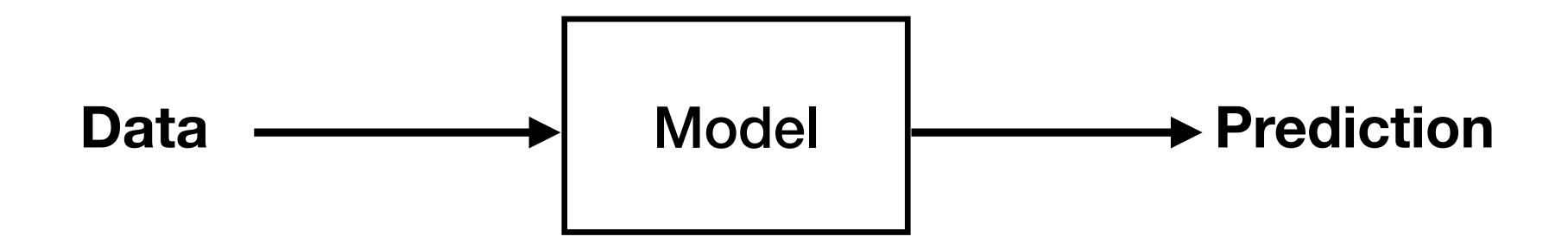
- Supervised Learning
- Unsupervised Learning
- Semi-supervised Learning
- Reinforcement Learning



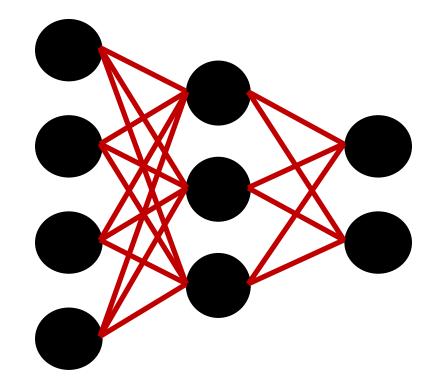
Examples from Systems

- Supervised Learning Performance models, Code completion tasks, etc.
- Unsupervised Learning Large code models (Github Co-pilot)
- Semi-supervised Learning
- Reinforcement Learning Code Optimization, Design Space Exploration

Machine Learning Simplified!



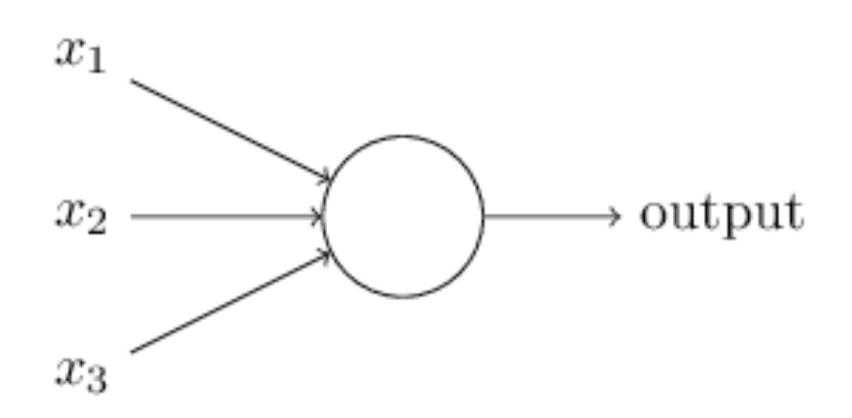
- Images
- Program Code
- Sentences
- Robot State



- Label
- Performance
- Translation
- Action

Possibly a Neural Network
(A non-linear function with tunable parameters)

Perceptrons



output =
$$\begin{cases} 0 & \text{if } \sum_{j} w_{j} x_{j} \leq \text{ threshold} \\ 1 & \text{if } \sum_{j} w_{j} x_{j} > \text{ threshold} \end{cases}$$

x_i - binary input / real input

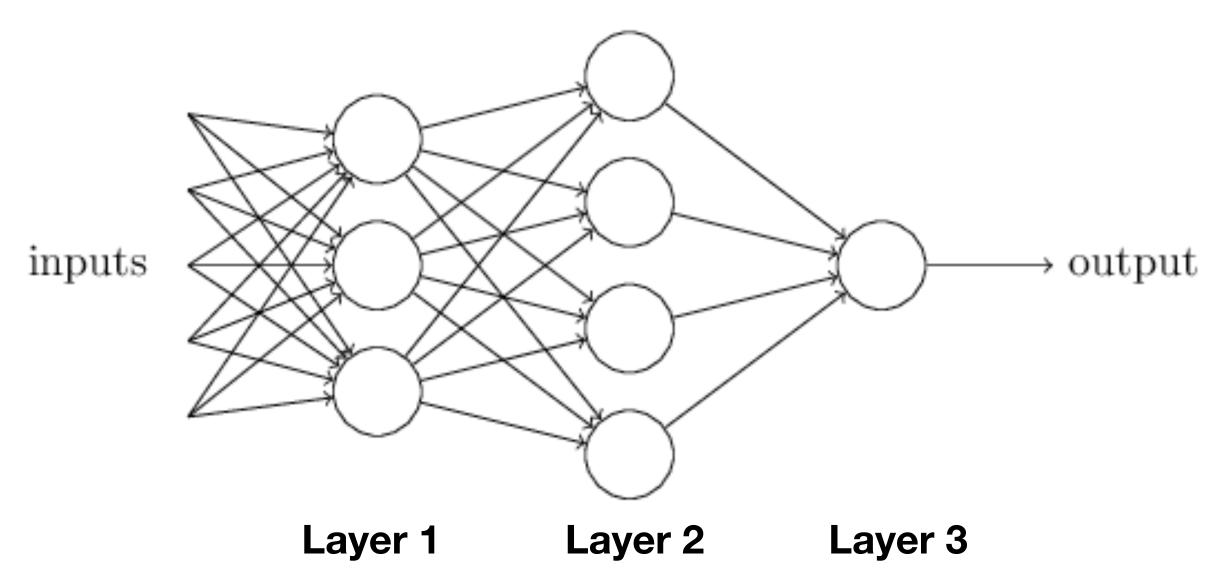
w_i - real weights

Output - binary output

Where's the non-linearity?

Can only separate linearly separable regions

Add more layers and perceptrons?



Is it more powerful than a single perceptron?

Now it is non-linear; yes

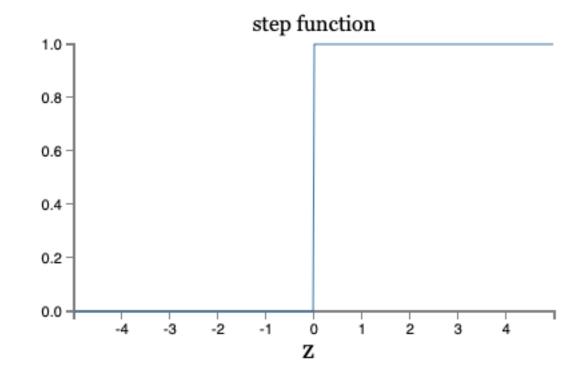
Each layer makes decisions about high-level concepts

How do we set the weights?

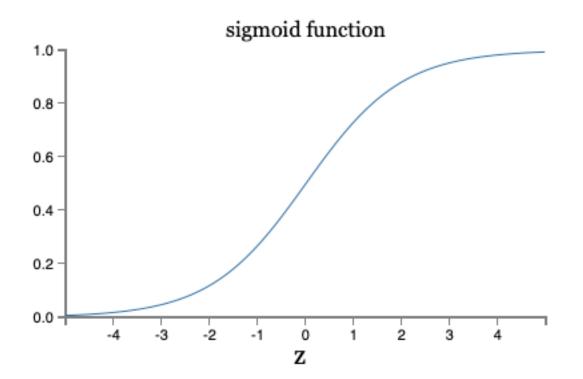
Let's devise an algorithm to learn them

Smooth Neurons

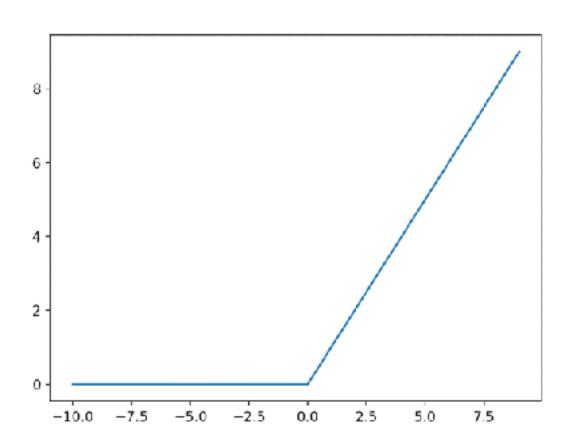
Instead of step function



Sigmoid Activations



Rectified Linear Unit Activations



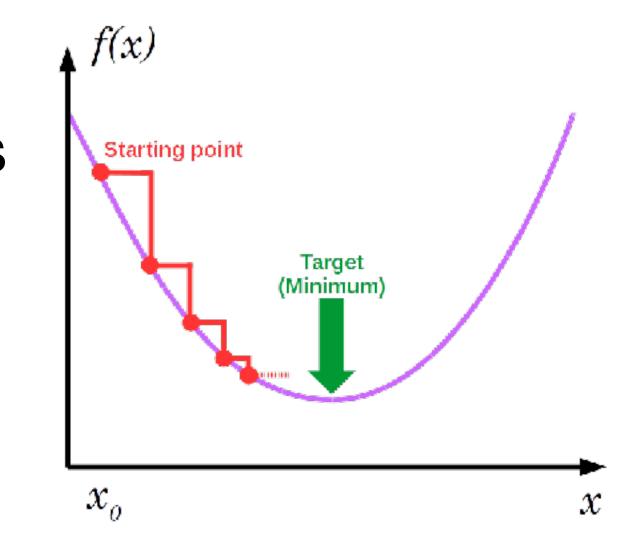
Learning

- The process of learning weights of each neuron connection
- Use gradient descent since NNs are differentiable

$$W_{i+1} = W_i - \eta \nabla F(W_i)$$
 η - Learning Rate

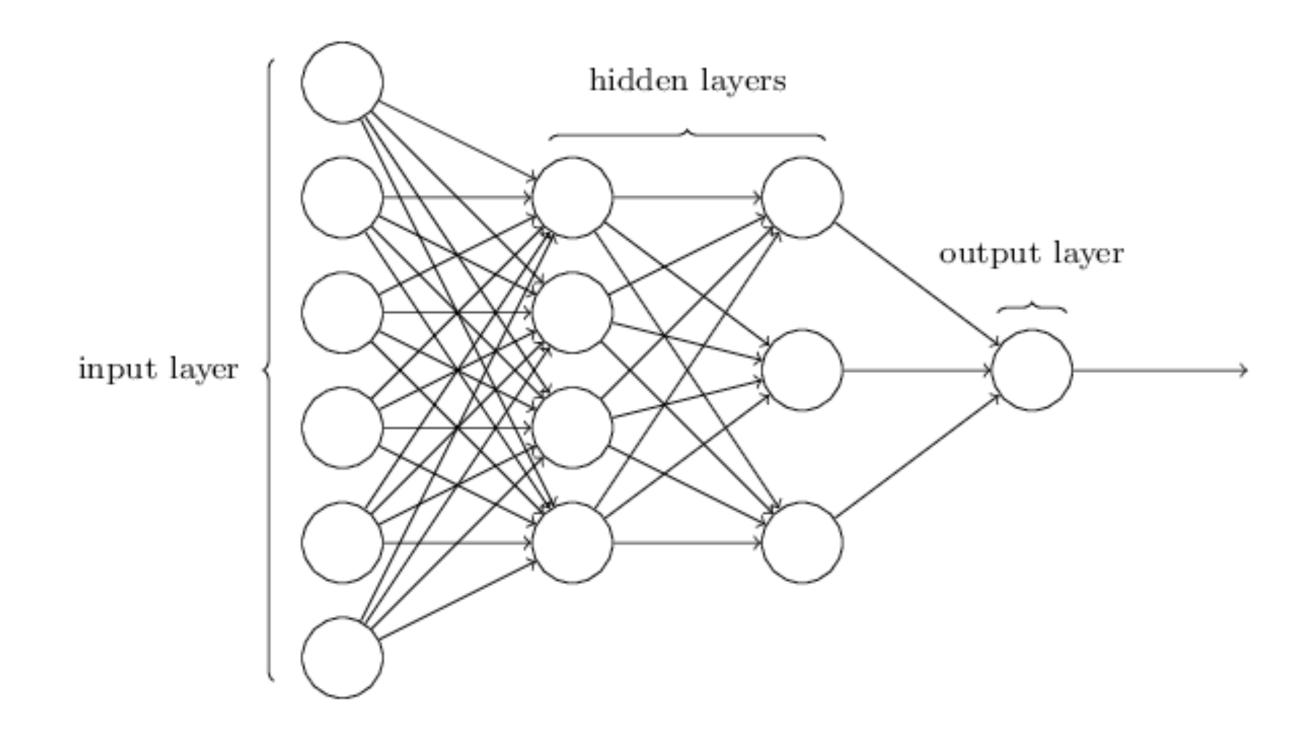
F(.) – Neural Network Function

 Use better variants with better convergence properties (e.g. Stochastic Gradient Descent, ADAM)



Multilayer perceptrons

- Same as Feedforward fully connected neural networks
- Uses smooth activations to build a multilayer connection of neurons



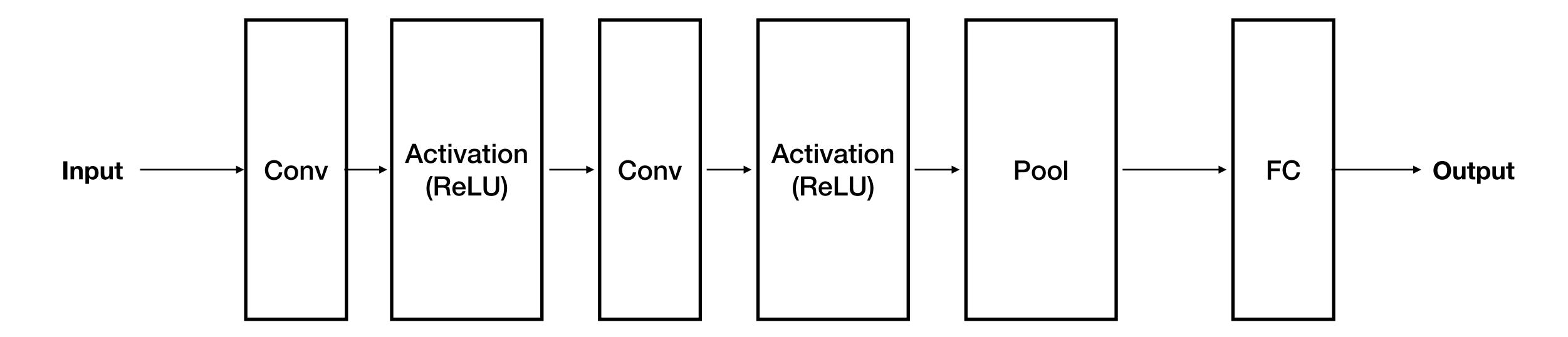
How powerful are NNs?

- Neural Networks are function approximations (differentiable)
- Do you need plenty of hidden layers to achieve more capacity?
 - Theoretically No: Universal Approximation Theorem
 - Informally, it says one hidden layer is sufficient to approximate any continuous function
 - It does not say about learnability (how to set the weights)
- In practice, different network topologies with deeper networks are needed to learn better approximations for problems at hand

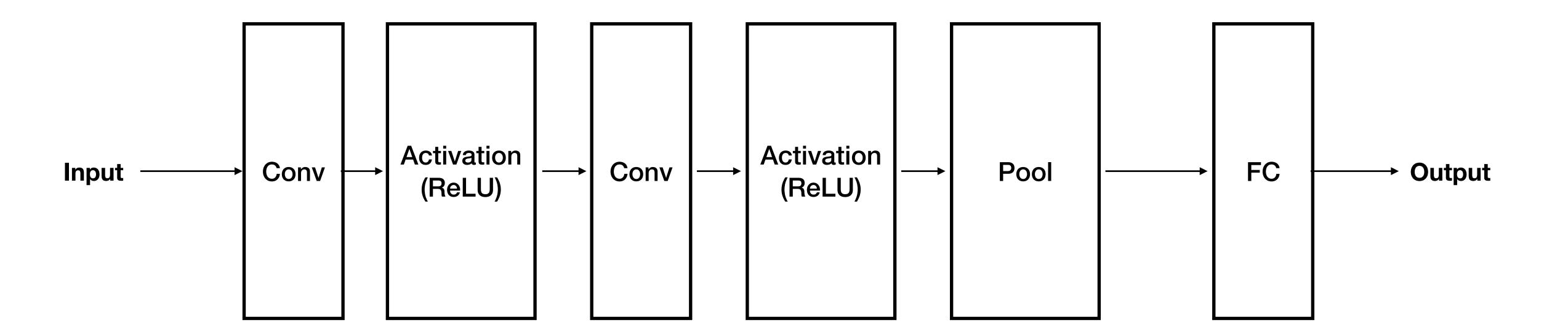
Quick Overview of Different NN topologies

Convolutional Neural Networks

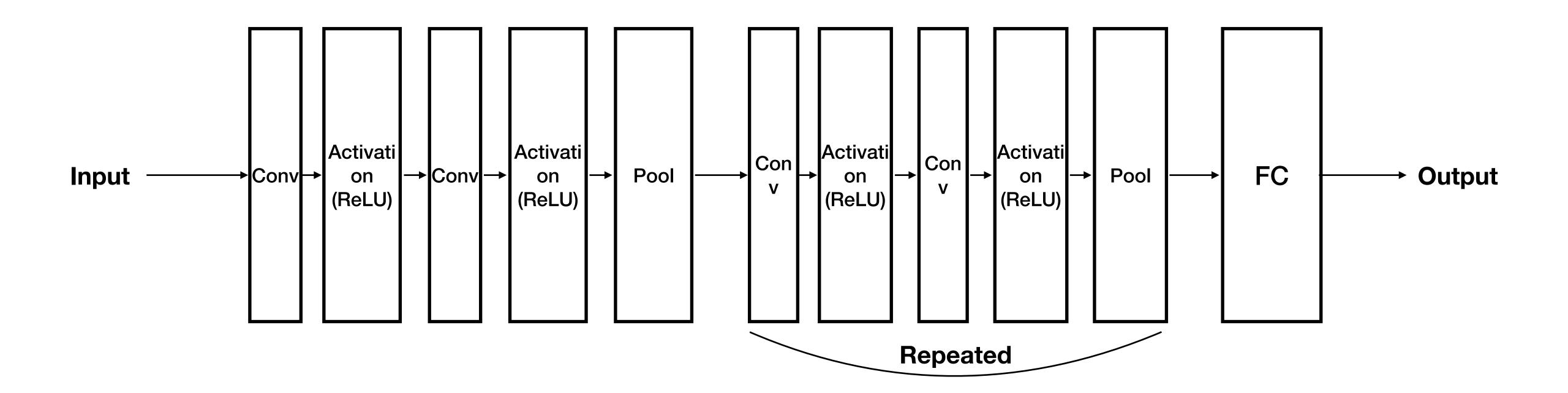
- Used in the image domain and mimics convolution filters on parts of the image
- Learnable parameters are weights of these convolution filters
- Usually have multiple convolutional layers and max pooling in between



Convolutional Neural Networks



Convolutional Neural Networks



AlexNet (2012)

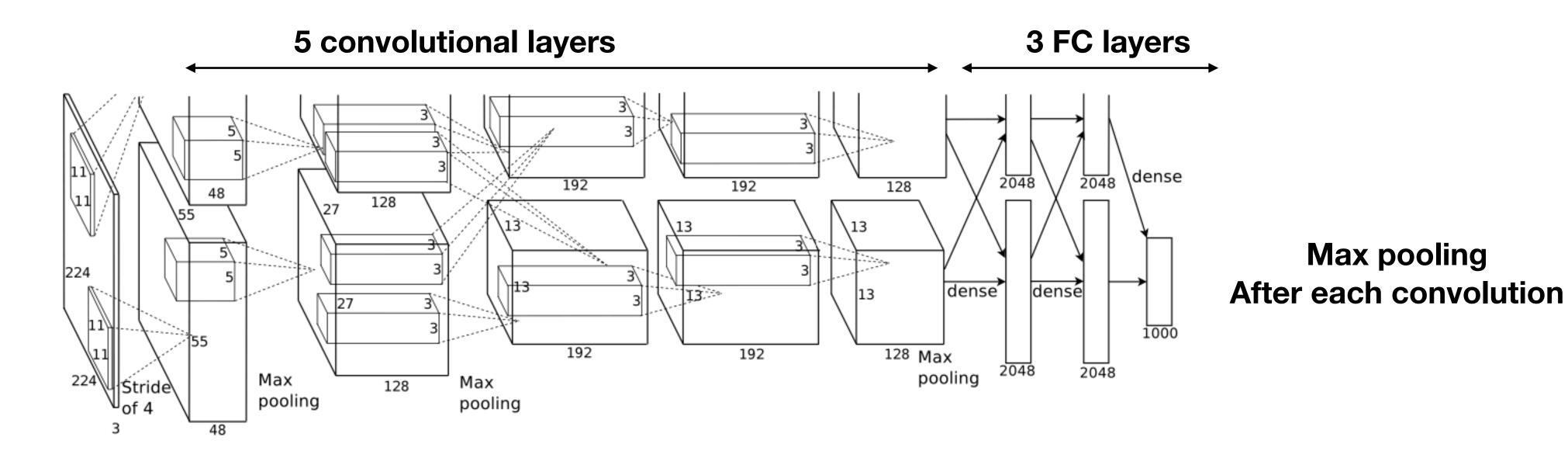
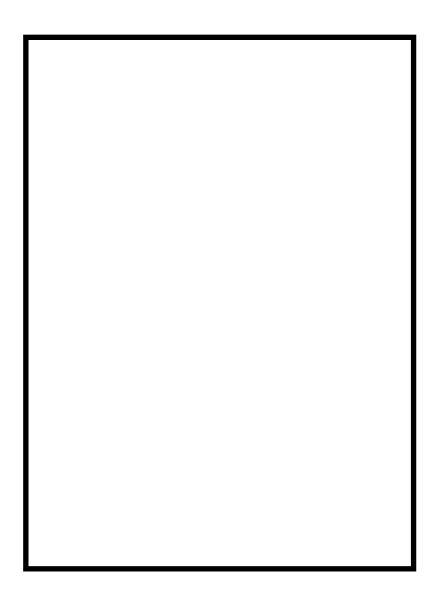


Figure 2: An illustration of the architecture of our CNN, explicitly showing the delineation of responsibilities between the two GPUs. One GPU runs the layer-parts at the top of the figure while the other runs the layer-parts at the bottom. The GPUs communicate only at certain layers. The network's input is 150,528-dimensional, and the number of neurons in the network's remaining layers is given by 253,440–186,624–64,896–64,896–43,264–4096–4096–1000.

What is a convolution?

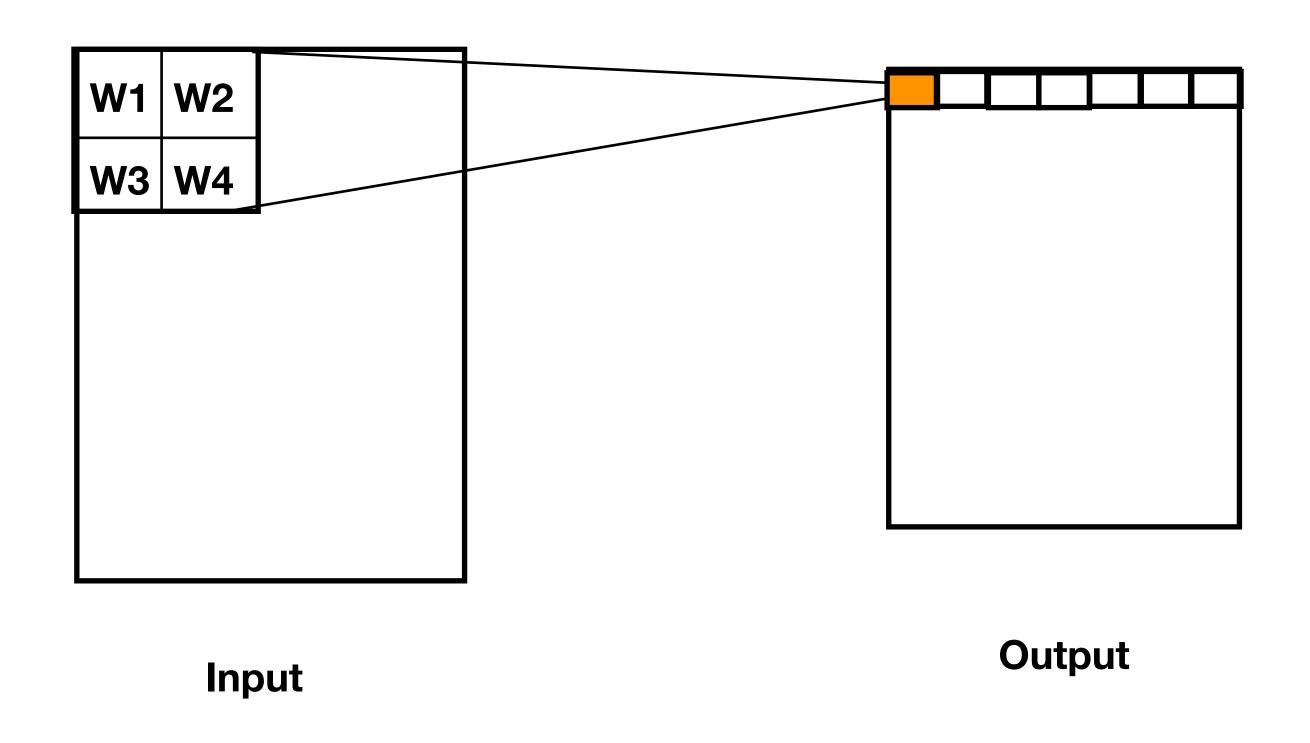


W1	W2
W 3	W 4

Kernel / Filter

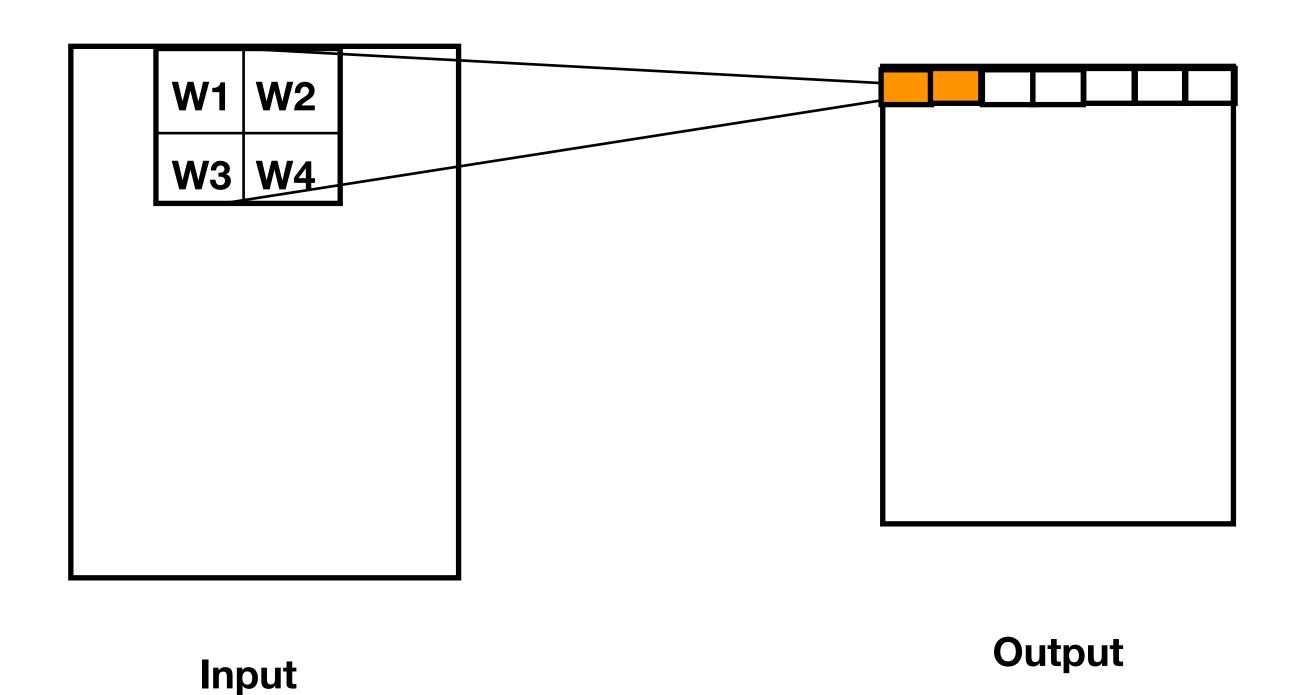
Input

What is a convolution?



Weighted sum of input values $\sum W_i x_i$

What is a convolution?

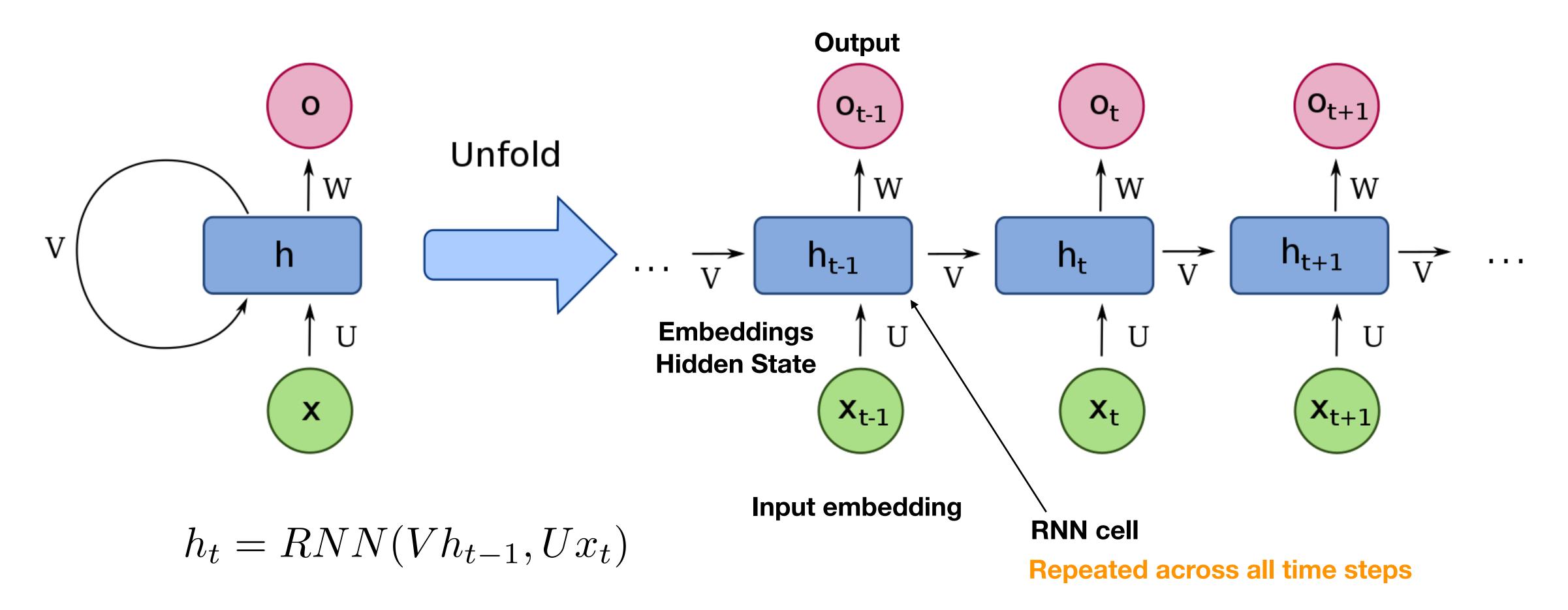


- 3D convolutions
- Depth-wise convolutions (grouped)
- Dilated Convolutions
- Padded Convolutions

Weighted sum of input values $\sum W_i x_i$

Recurrent Neural Networks

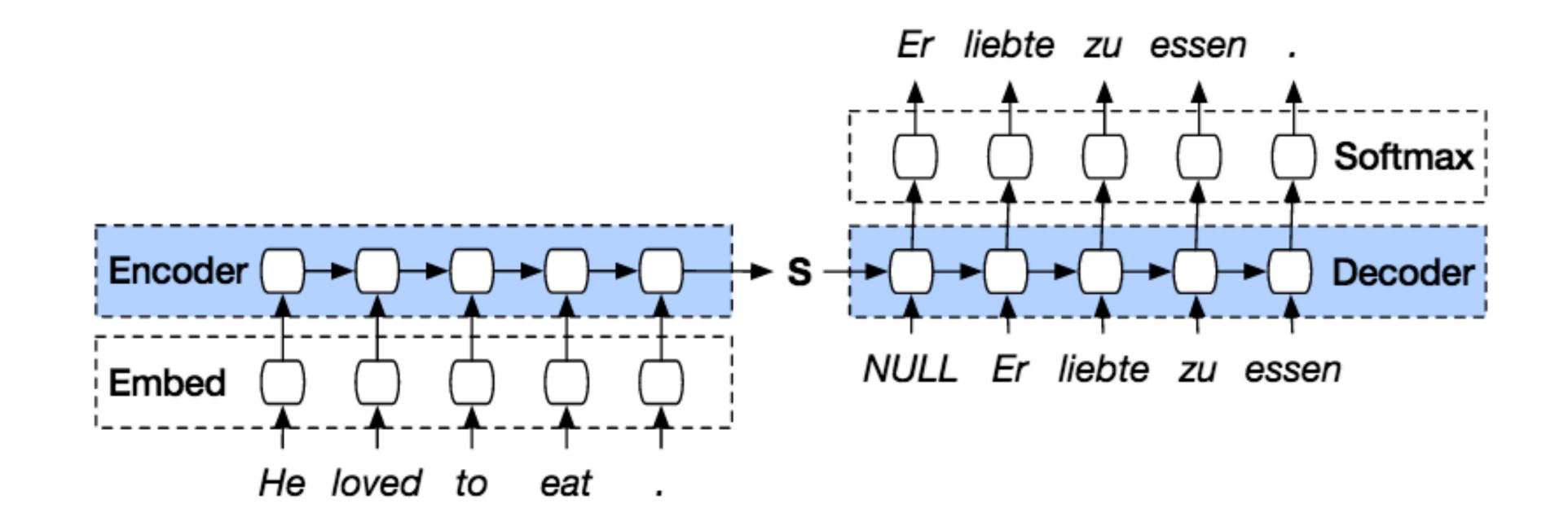
Neural network topology with history



Recurrent Neural Networks

- Main use case: when you need to remember across time steps
- Two main problems with training vanilla RNNs
 - Handling long term dependencies can be tricky
 - Vanishing or exploding gradients during training
- Two types of popular RNN cells that alleviate these problems
 - Long Short Term Memory cells and Gated Recurrent Units (https://colah.github.io/posts/2015-08-Understanding-LSTMs/)

Use case: Machine Translation



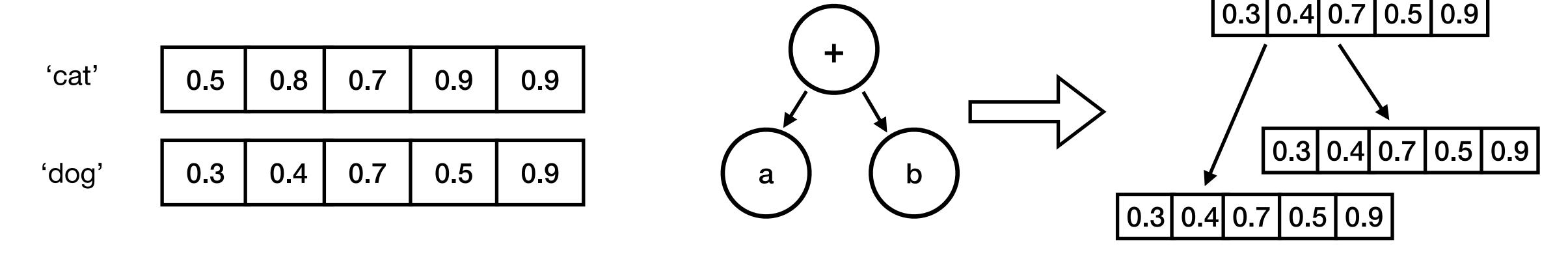
Graph Neural Networks

Works on graph structured data

Word Embeddings

 Main goal is to find representations for nodes or edges (node or edge embeddings) that can be used for many downstream tasks

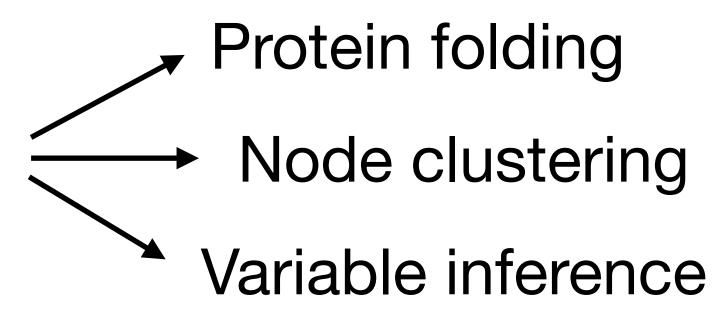
Embeddings



Node Embeddings

Graph Neural Networks

Find node embeddings for



Protein Interface Prediction using Graph Convolutional Networks

Alex Fout[†]

Department of Computer Science Colorado State University Fort Collins, CO 80525 fout@colostate.edu

Basir Shariat†

Department of Computer Science Colorado State University Fort Collins, CO 80525 basir@cs.colostate.edu

Jonathon Byrd[†]

Department of Computer Science Colorado State University Fort Collins, CO 80525 jonbyrd@colostate.edu

Asa Ben-Hur

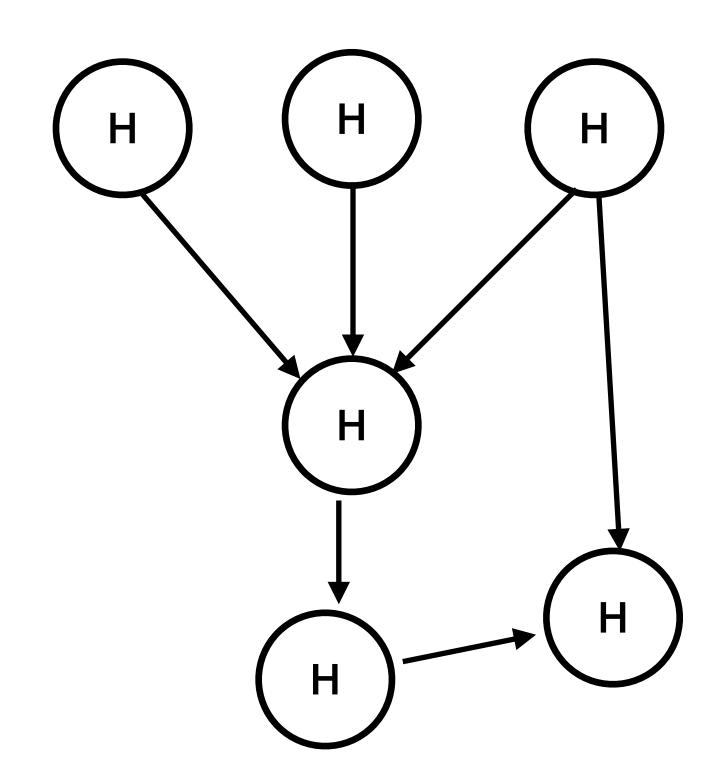
Department of Computer Science Colorado State University Fort Collins, CO 80525 asa@cs.colostate.edu

Spectral Clustering with Graph Neural Networks for Graph Pooling

Filippo Maria Bianchi * 1 Daniele Grattarola * 2 Cesare Alippi 2 3

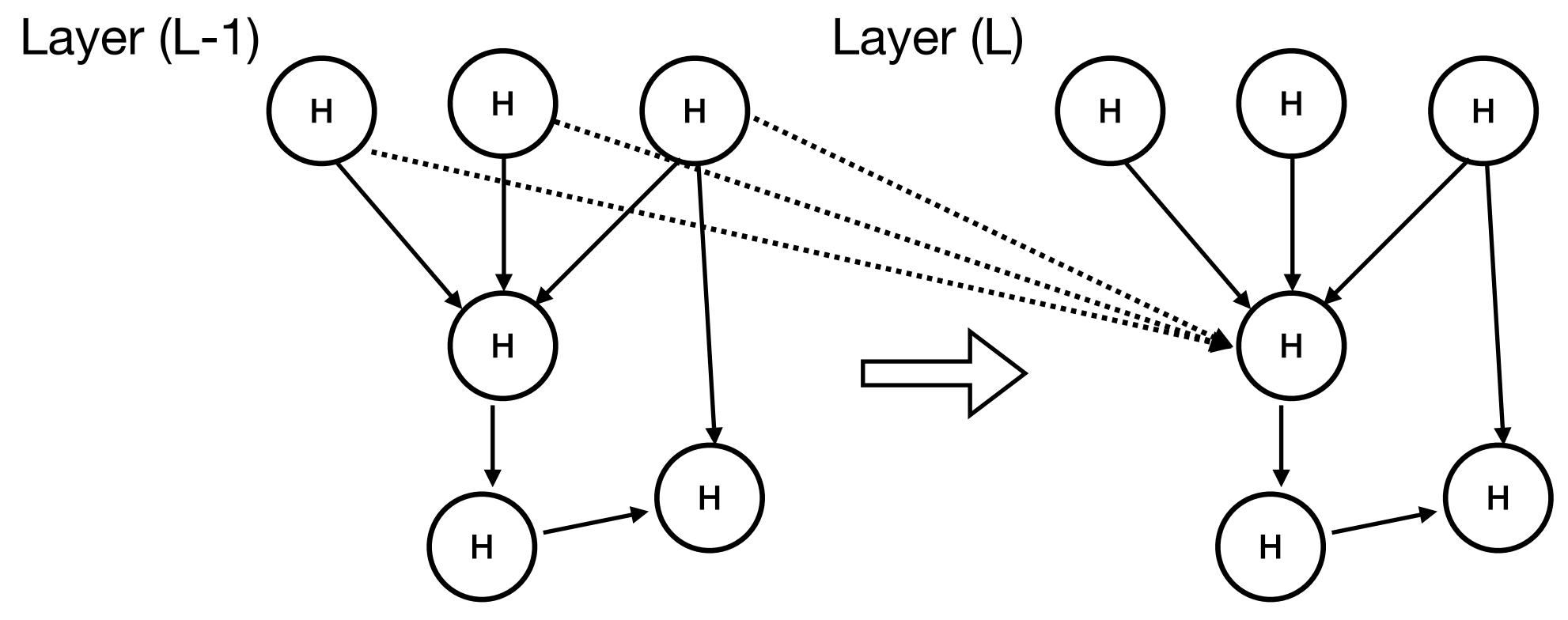
Predicting drug-target binding affinity with graph neural networks

Thin Nguyen, Hang Le, Thomas P. Quinn, Thuc Le, Svetha Venkatesh doi: https://doi.org/10.1101/684662



Computational Model

All nodes are updated at layer (L) from layer (L-1) values in parallel Style

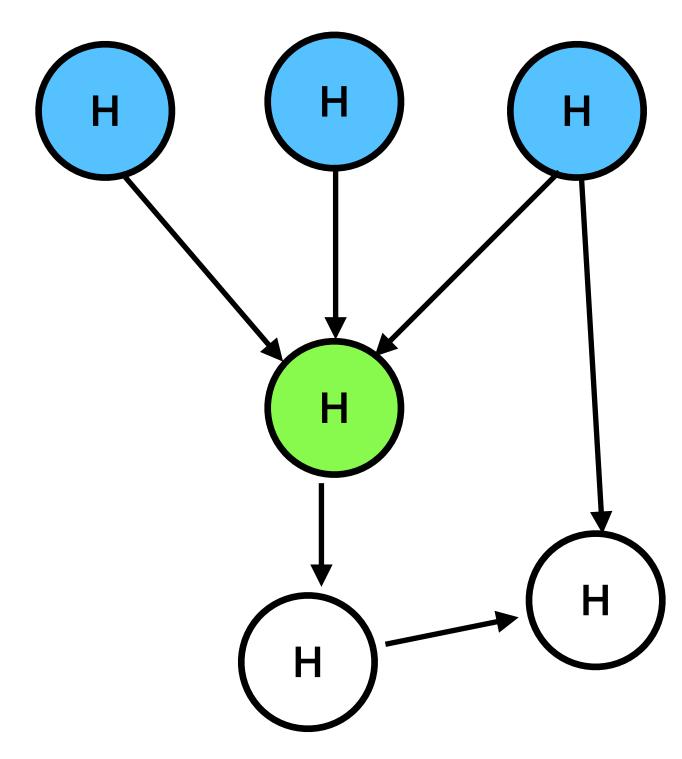


Computational Model

Bulk Synchronous Parallel Style

All nodes are updated at layer (L) from layer (L-1) values in parallel

Updates from a neighborhood of nodes (message passing)



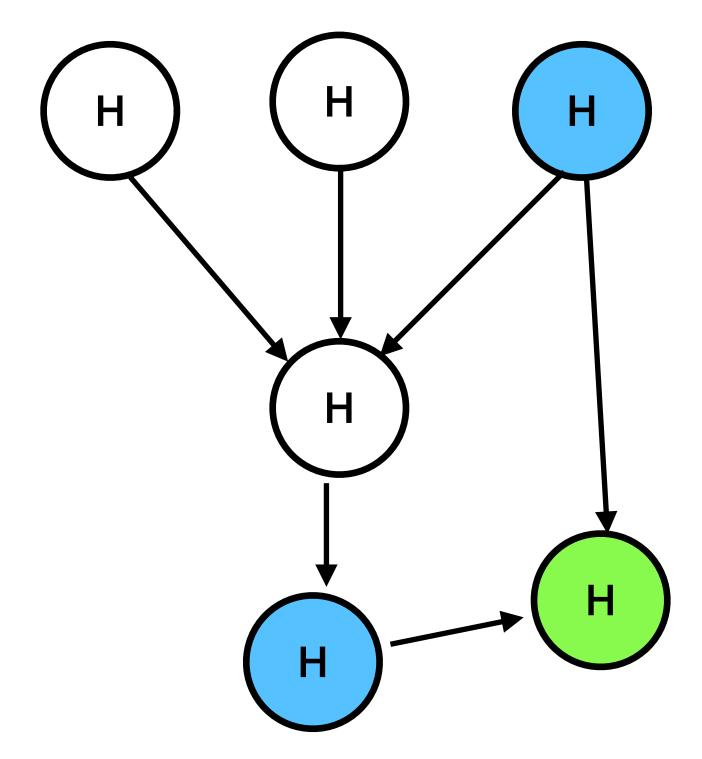
Computational Model

Bulk Synchronous Parallel Style

All nodes are updated at layer (L) from layer (L-1) values in parallel

→ Updates from a neighborhood of nodes (message passing)

Barrier until all nodes are updated



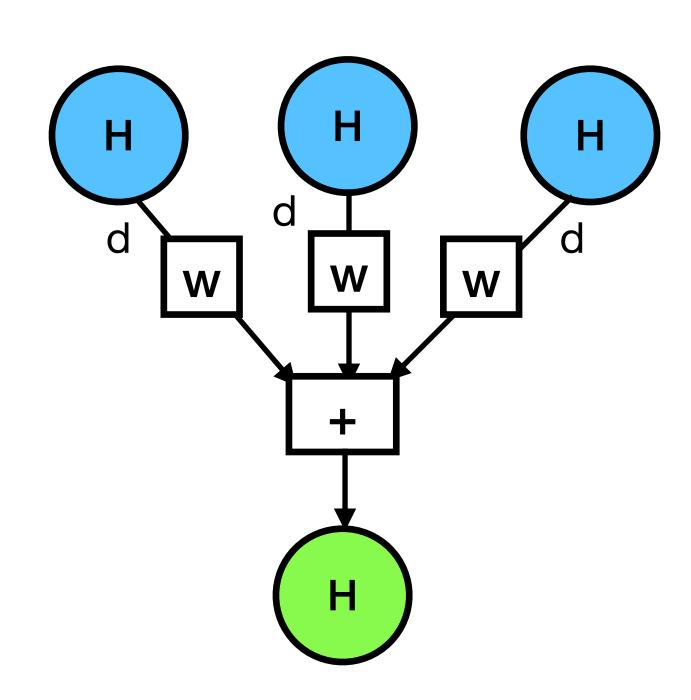
Neighborhood

Message

Aggregation

Update

Graph Convolutional Network (GCN)



Suitable for Transductive Tasks

Neighborhood = All single-hop

Message Fixed importance $d = \frac{1}{\sqrt{d_{ii}d_{jj}}}$

Learnable Weights W(l)

$$dh_u^{(l)} \cdot W(l)$$

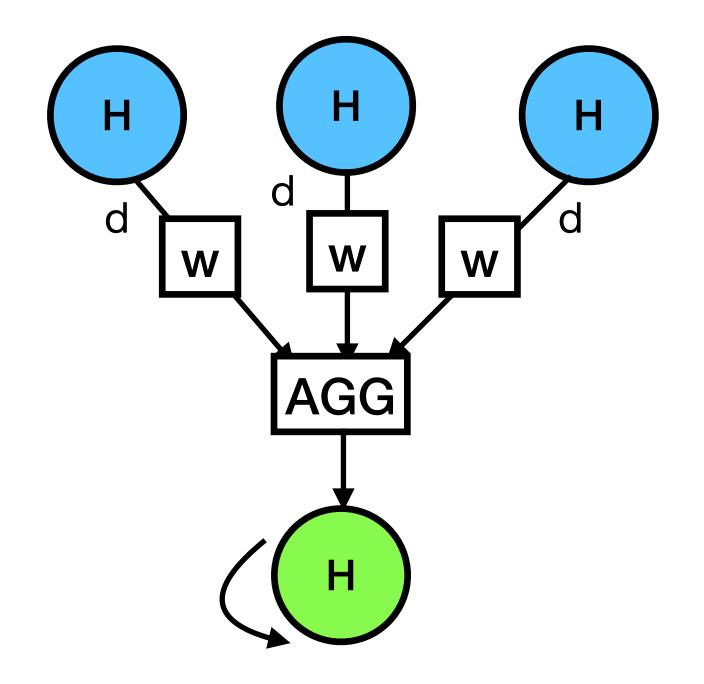
Aggregation Sum (fixed)

Update

$$h_v^{(l+1)} = \sigma \left(\sum_{u \in ne(v)} \frac{1}{\sqrt{d_{ii}d_{jj}}} h_u^{(l)}.W(l) \right)$$

GraphSAGE

Generalization of GCN



Suitable for Inductive Tasks

Neighborhood = All single-hop

Message Fixed importance d=1

Learnable Weights W(l)

Subsample nodes

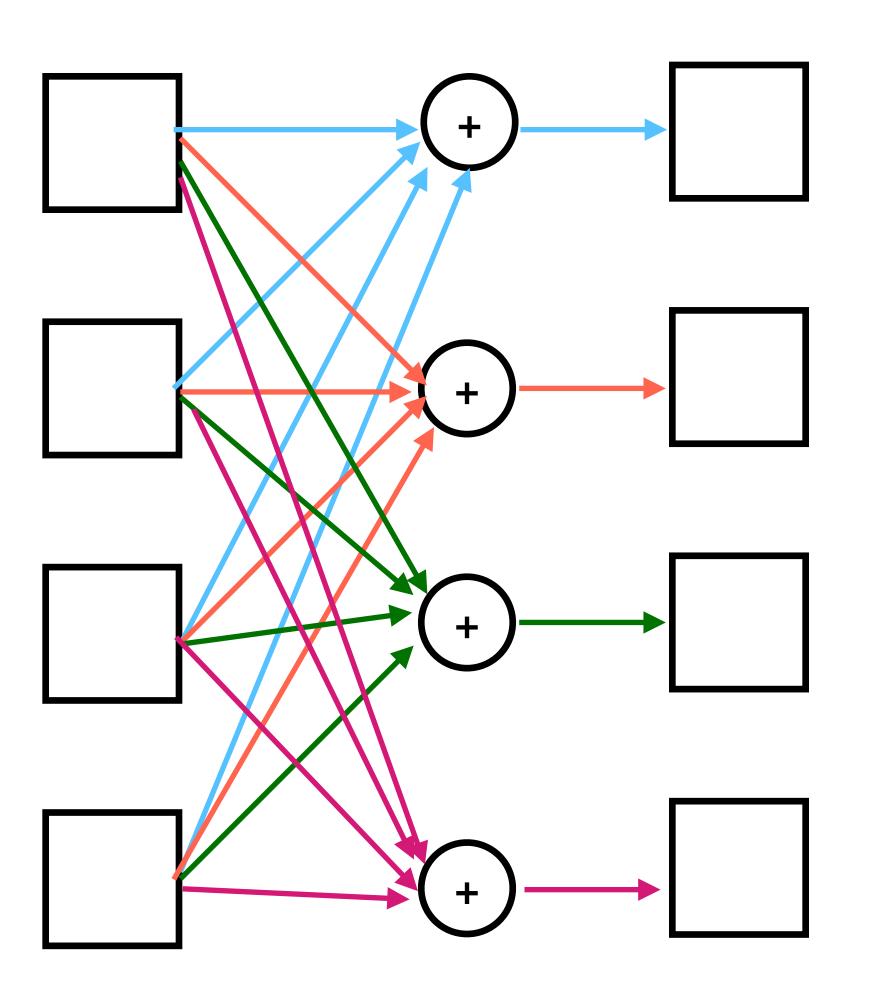
Aggregation +, pool, LSTM

Update (concatenate current node embedding)

$$h_v^{(l+1)} = \sigma\left(\left(h_v^{(l)}||AGG(h_u^{(l)}|u \in N(v))\right).W^{(l)}\right)$$

Inductive Representation Learning on Large Graphs (NeurIPS 2017)

Transfomers Primer



Easily parallelizable and can distribute work

Function Approximators

- Neural networks are non-linear function approximators
- We usually use gradient based techniques to learn the parameters (weights)
 - Other techniques can be used as well
- Can be used to approximate many parts of a system
 - Policy of a moving robot
 - Image classification system
 - Machine Translation
- Novelty comes from designing new topologies and adapting your system to use NNs.

Next Lecture

- Genetic Algorithms
- Reinforcement Learning basics
- Auto-tuning and Design Space Exploration

Any Questions?