EECS 182/282A

Today: Finish GNN: Pooling
Start RNNs

Reading: Prince through Ch 11 + Ch 13
Note: Nothing in this lecture is in the Prince textbook.
Older RNN material: deeplearningbook.org
Project Info Coming Today. Keys: Required Meeting: Oct 27–
Proposal: Nov 3rd
Required Meeting: Nov 3–

Architecture Order In Class:

MLPs → CNNs → Graph NN → RNN/state-space → Transformers

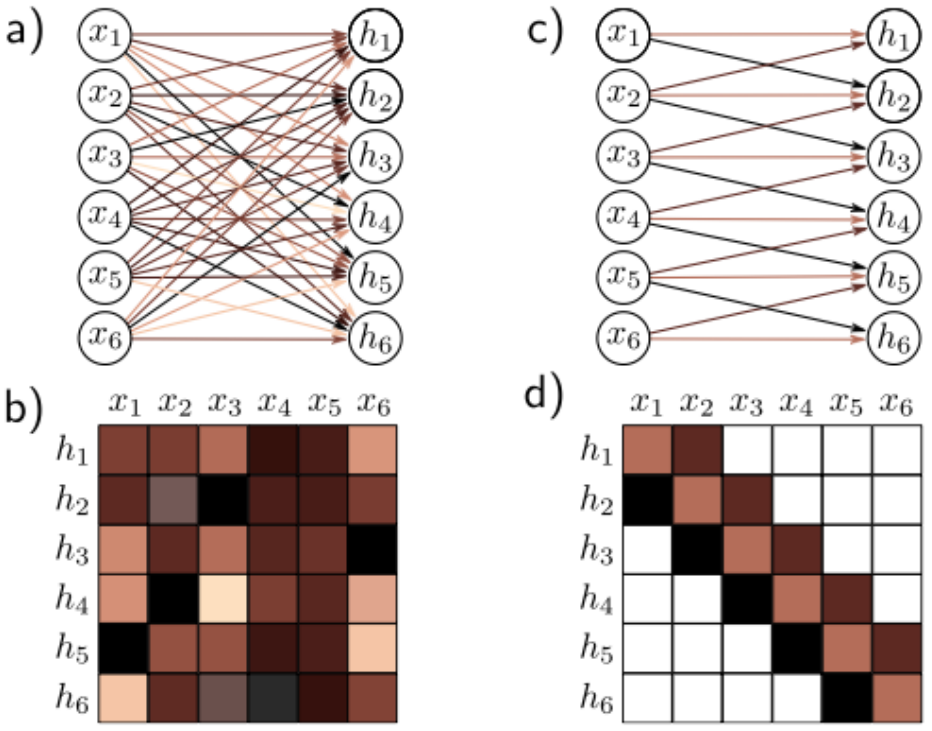
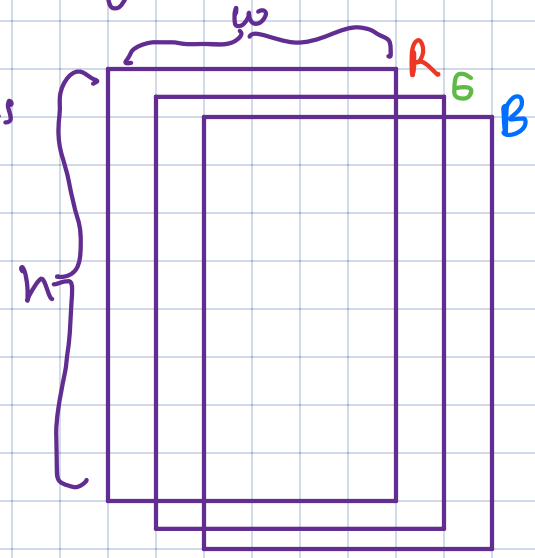


Fig 10.4 in Prince

MLP CNN

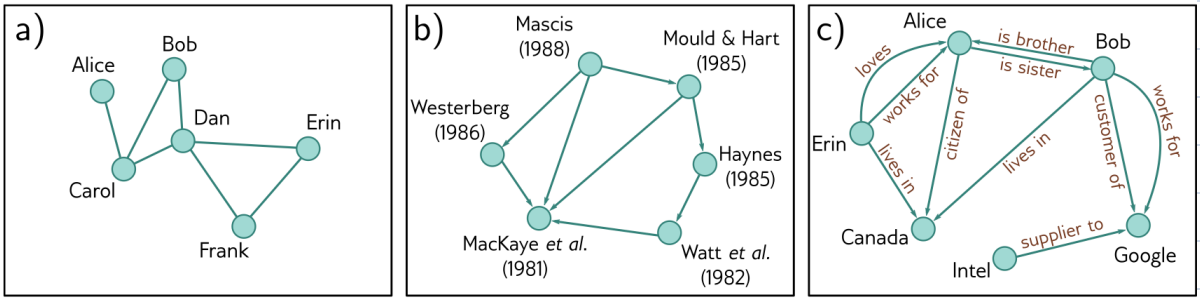
Inspired by computer vision problems: classification,

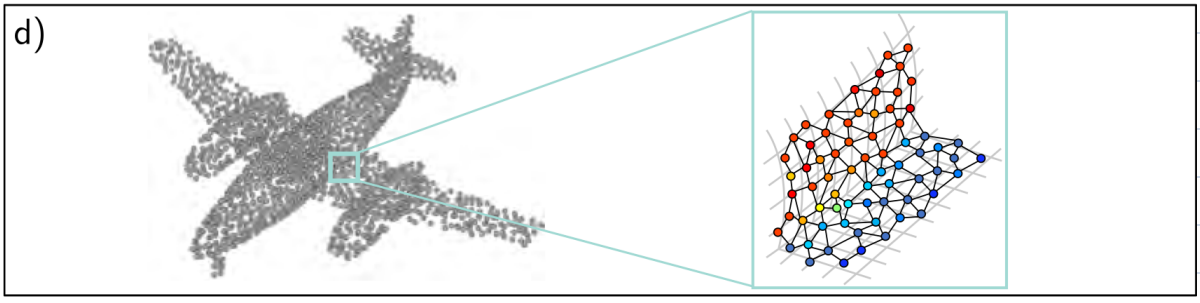


$h \times w \times 3$ ← channels c

semantic segmentation, etc.

Generalizing CNNs: Images → General Graphs





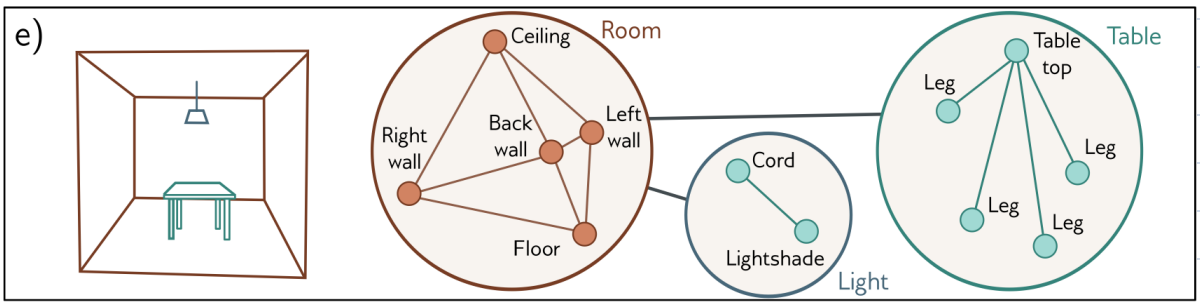


Fig 13.2 in Prince

Image Classification

Semantic Segmentation

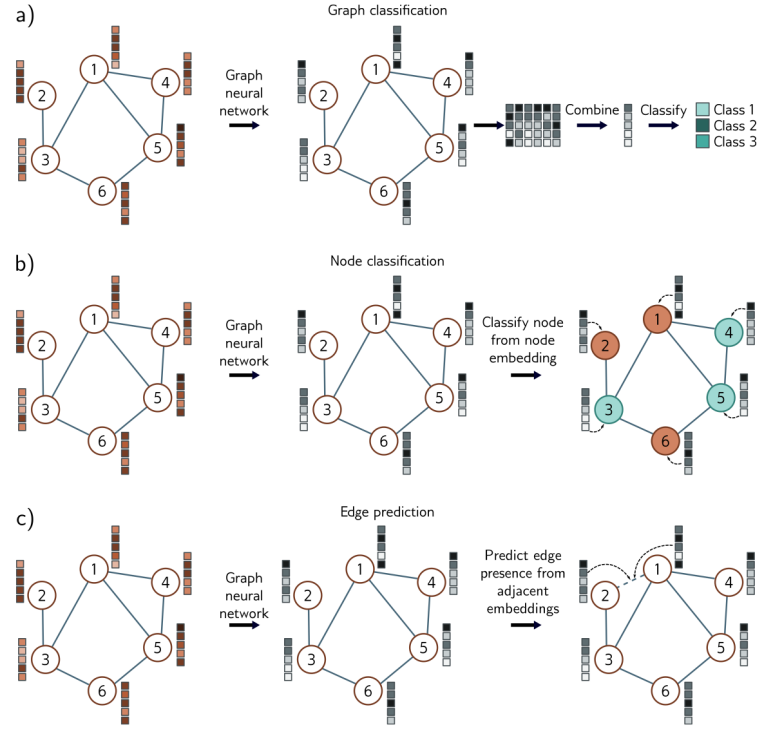
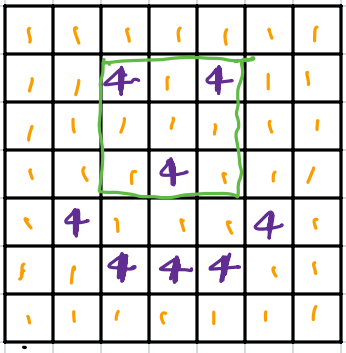
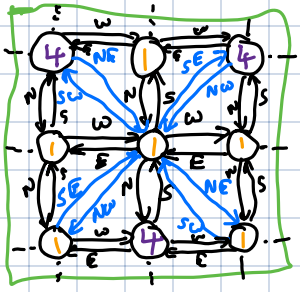


Fig 13.6 in Prince

First Conceptual Step: Image as a graph

Nodes = Pixels





Directed Graph

Edges labeled with one of

{N, S, E, W, NE, SE, NW, SW}

(Always a special relation to self)

A 3×3 Conv can be viewed as receiving messages from neighbors, each of whom has their own labeled edge to me, multiplying by an edge-label-specific weight matrix, and adding those up together with a special self-specific matrix acting on this node's info and a bias $\vec{b}$.

Note: Implicit Zero-Padding and Same-Pad Weight-sharing across nodes

1×1 Convs are local to a node

Matrices W_i and biases $\vec{b}$ are specific to layer of processing

Recall Picture:

3×3 example:

W_{NW}	W_N	W_{NE}
W_W	W_{me}	W_E
W_{SW}	W_S	W_{SE}

C_{out} $\{ \overbrace{W_i}^{C_{in}}, \vec{b} \}$ C_{out}

$$\vec{h}_{out} = \vec{b} + \sum_i W_i \vec{h}_{in,i}$$

Taking Stock: We have, in principle, an immediate recipe to generalize CNNs to directed graphs with the same property: Every edge labeled from a discrete finite set.

What Generalizes Immediately: Weight-sharing (Nodes do the same things)

3×3 convs (As above, Matrices for edge-labels)

Additional Channels, Residual Connections, Dropout for MLPs, Stochastic Depth,

What does not generalize: Pooling / Downsampling and Upsampling

What needs discussion: Normalization.

Core Insight: The graph plays the role of the empty grid of pixels in CNNs. The input is a graph with vectors in it

What does not generalize: Pooling / Downsampling and Upsampling

Key Challenge

Why do we pool anyway? — Grow Receptive Fields Faster (with layers)

Hack for GNNs: Add a fake global node connected to everything.

Aside: "Oversquashing" — information from far away lost because of small embeddings.
vs "oversmoothing" — the operations of the GNN naturally blur away all fine-grained details

Is there a way to go: Many → Few based on vector contents?

Like Clustering!

Recall Classic Clustering Approach: k-means / Lloyd's Algorithm for VQ

Hyperparam Choice: k

0) Start at random in some way

1) Calculate Centers

2) Map points to centers to get clusters

3) Goto 2 & Repeat

Is this differentiable? No.

What's the barrier? Hard Assignments of points to clusters

Can we use a softmax or something like that?

DiffPool Idea: When we downsample, we get a smaller graph but it's fully connected with probabilities on each edge

[Good Docs in PyG]

Hierarchical Graph Representation Learning with Differentiable Pooling by Ying, et al. 2019

Make each point belong to every cluster, just with some probability.

"Grey-box" the problem: Input: Graph with Embedded Vectors

Output: k-length vector for each node with probabilities in it

i.e. $s_i^T = [p_1, \ldots, p_k]$ for node i

Need differentiable operation that does this.

Ingredients? 1) Softmax on scores will give me

New Problem: Given a graph, do some differentiable steps to get scores.

Don't know what to do. Make it learnable.

What's a generic way to have a learnable algorithm on a graph?

USE a GNN!

Wherever we need to "downsample" a graph insert a little GNN that doesn't share weights with the rest of the GNN and has the structure:

But these $\vec{s}_i^T$ aren't a graph... Not yet.

What do we do with these soft assignments to clusters?

Need New Vectors (Embeddings) for the k clusters.

$$\vec{h}_j^{(l+1)} = \sum_i S_i[j]\, \vec{h}_i^{(l)}$$

- j^{th} cluster in layer $l+1$ (After Pooling)
- i: Pre-Pooling nodes
- $S_i[j]$: "Probability" node i belongs to cluster j

The content of original node flows into different cluster according to membership

Need New (Soft) Adjacency Matrix

$N\{A^{(l)}$ ← original adjacency (symmetric Matrix)

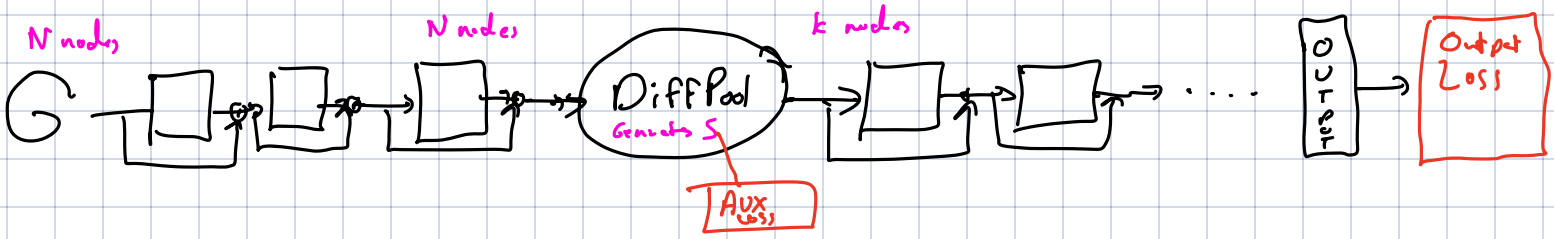
$$k\{A^{(l+1)} = k\{S^T A^{(l)} S\}_N$$

where $S = \begin{bmatrix} S_1^T \\ S_2^T \\ \vdots \\ S_N^T \end{bmatrix} \}N$ (k columns)

So A_{ij} represents how strong the edge is between cluster i and cluster j

Now we have a new graph! With k nodes and a new Adjacency Matrix

Put things together



Can Train end-to-end. But we can do better.

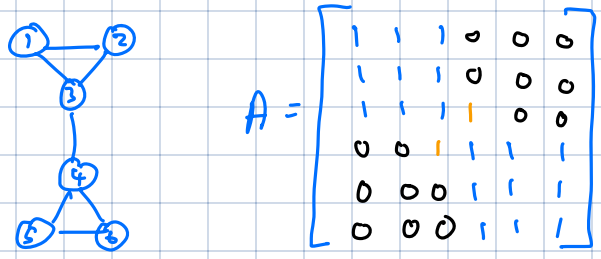
Auxillary Losses can help get desirable properties.

Note: When passing activations across one of these edges, can multiply by A_{ij} to account for the strength of the edge. [Important therefore to not immediately normalize these messages]

Property 1: Have clustering respect graph topology

$$\| A - {}^{N}S^{k}{}^{k}S^{T} \|_F$$

What kind of information does this encourage in the embeddings?



${}^{N}S^{k}{}^{k}S^{T}$ has low-rank structure

That's what we want from the example here

Note: The entries in SS^T are pairwise inner products of the $\vec{s}_i^T$ with $\vec{s}_j^T$.

Property 2: Want to be close to hard cluster assignments

$$\frac{1}{N} \sum_i H(\vec{s}_i^T)$$

Probabilities

Entropy minimized by $[0, 0, \ldots, 1, 0, \ldots 0]$

Note: Hyperparameters: weights for Aux losses. Follow what others do...

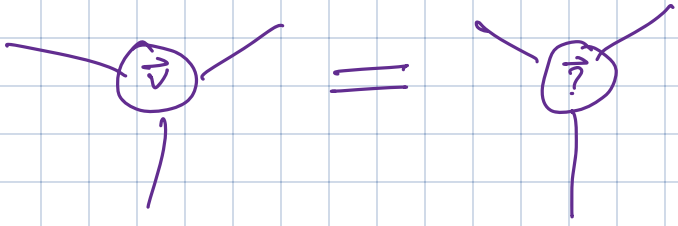
	Edge Labels (finite)	Edge Labels (infinite)	None
Directed	✓ Like CNN		
Undirected		DiffPool results in weights on edges (in particular scalars)	✓ without Pooling

Final Challenge: Held-Out Data (Node-level Problems)

Approach 1: Excise entire nodes from the graph.

Challenge: Impacts connectivity

Approach 2: Remove content from the node but leave it in.



$\vec{?}$ = learnable vector
usually called $\vec{\text{mask}}$

Note: (From Office Hours)

By making $\vec{?}$ learnable, we need to make sure the training examples seen during training let that happen.

There are two desiderata from $\vec{?}$:

1) It shouldn't impede information flow as messages are passed. ← This will happen even with the $\vec{?}$ in truly held-out positions during training.

2) It should prompt the network to correctly predict labels for the node even though there isn't input there.

To get (2) to happen, it is useful to do data augmentation during training. Randomly mask some nodes for which we have target labels, and keep the loss on that node's predictions.

RNNs: Recurrent Neural Nets

History: Before 2018, concensus view: Two big successes in NN:
Images & Vision using CNNs
Language & Speech using RNNs

Key issue in language & speech (along with control, time-series, etc.) sequential data

A signal-processing perspective

SP	Neural Nets	Weight-sharing
FIR Filter (finite impulse response)	CNN	Across Space
IIR Filter (infinite impulse response) Finite-dimensional hidden state inside filter. Sequential & Causal	RNN	Across Time

Approach: Keep all the design ideas & principles from CNNs.
Just replace space with time and enforce causality.